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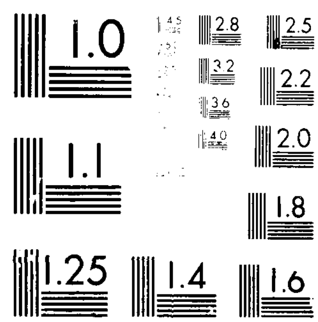

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Report No. FAA-EE-80-11

HIGH ALTITUDE POLLUTION PROGRAM STRATOSPHERIC MEASUREMENT SYSTEM LABORATORY PERFORMANCE CAPABILITY REPORT CHEMICAL CONVERSION TECHNIQUES

LEVEL II

ADA085198

Norman H. Macoy and Richard Weingarten
with
Anthony Pires and Sherman Poultney

February 1980
TECHNICAL REPORT

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Prepared for
HIGH ALTITUDE POLLUTION PROGRAM

U.S. DEPARTMENT OF TRANSPORTATION
FEDERAL AVIATION ADMINISTRATION
Office of Environment and Energy
Washington, D.C. 20591

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16. Abstract
This report documents the laboratory measurements made to resolve specificity questions concerning the chemical conversion techniques for measurement of stratospheric trace species NO_2, N_2O_5, and HNO_3 to NO (which is the measurable species). Particular emphasis was placed on the conversion of NO_2 to NO by both catalytic and photolytic converters, thermal conversion of N_2O_5 and HNO_3 to NO_2 with and without possible interfering gases, and the feasibility of measuring total odd-nitrogen concentrations using catalytic thermal conversion to NO. The laboratory measurements were generally carried out at ppm concentrations at STP conditions. The GEARS/EPISODE computer code was used to model both the laboratory reactions and the behavior of the technique at stratospheric conditions. The laboratory measurements and stratospheric simulations lead to the recommendation to develop a flight prototype of a Hybrid Gas Conversion System consisting of a number of instrumentation modules. The first module would be a Total Odd-Nitrogen module (and NO) based on high temperature catalytic conversion of the odd-nitrogens and chemiluminescent detection of NO. The second module would be an NO_2/NO module based on NO_2 photolysis and NO chemiluminescent detection. Other modules could consist of an O_3 UV photometer, an N_2O gas chromatograph, and other appropriate modules that are ready at flight time.

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SECTION I

INTRODUCTION

This report documents the laboratory measurements made to resolve specificity questions concerning the Hybrid Chemical Conversion Measurement System and to examine the potential of a conversion technique for total odd nitrogen, as recommended in the High Altitude Pollution Program (HAPP) Stratospheric Measurement System Feasibility Study. That study and these laboratory measurements are part of a large study of the High Altitude Pollution Program Stratospheric Measurement System being done by the Perkin-Elmer Corporation for the Department of Transportation, Federal Aviation Administration under Contract DOT-FA77WA-4080. The goal of this larger study is to define and demonstrate a measurement system consisting of a technique or combination of techniques that can be flown on a series of balloon flights to make prescribed, *in situ* measurements of the stratosphere in support of the High Altitude Pollution Program. The other components of the total study include the feasibility of the Tunable Diode Laser Spectrometric System for the prescribed measurements, detailed engineering design documentation for the recommended payload, and a summary report. These other components of the study will be reported separately.

The Feasibility Study (Macoy et al., 1978) had concluded that the feasibility of successfully developing and flying a balloon-borne measurement system was high, based on a careful examination of the candidate system from an engineering point of view. The Study recommended that the system, consisting of a hybrid of analytical techniques, should be developed and deployed pending resolution of certain specificity questions. The selection of the Hybrid Chemical Conversion System was based on a comprehensive and critical review of all measurement techniques. This review included molecular chemical conversion, atomic chemical conversion, ion molecular conversion/mass spectroscopy, *in situ* optical absorption gas chromatography, and resonance fluorescence. Only the Hybrid Chemical Conversion techniques were to be appropriate

for an on-station balloon payload and within current state-of-the-art technology. Even then, certain of these techniques were subject to questions of conversion specificity. The questions did not invalidate those techniques, but might place several prescribed species into one class. The resolution of the specificity questions was therefore necessary and that work is one of the subjects of this report.

As the Feasibility Study was concluding, it became evident that progress in each of the reviewed techniques was not standing still and certain promising techniques should continue to be investigated in parallel to the resolution of specificity questions. The promising techniques were the Tunable Diode Laser Absorption Spectrometer and the Total-Odd Nitrogen Converter. The latter might turn the very lack of specificity of the conversion techniques into a capability to make the important measurement of total odd-nitrogen in the stratosphere. The study of the potential of this converter is another subject of this report. The Tunable Diode Laser Spectrometer technique gave promise that it might be able to measure all of the prescribed species if the IR signatures of heavier molecules cooperated and the requisite S/N performance could be achieved in the field. The study of the feasibility of a Tunable Diode Laser Spectrometer Measurement System is reported in a separate report (Poultney et al., 1979).

As this report is being written, progress in the reviewed techniques is still being made and the list of prescribed species is being re-examined. The ability to take advantage of advances in measurement capability is one great strength of the hybrid system that is recommended. A new technique can replace or supersede a weaker technique in the hybrid system without making the whole system obsolete. One new technique under development in the community for NO_2 promises to increase the feasibility of the Hybrid Gas Conversion system in that manner. This new technique and its potential impact on the realization of the HAPP Stratospheric Measurement System is also addressed in this report. A second strength of the Hybrid System is the ability to add or delete species (or parameters) without making the whole system obsolete. Instruments are being developed to measure these new species and parameters and could be later included in the Hybrid System. We do not here review any of these new instruments (e.g. a J_{NO_2} instrument).

The originally prescribed measurements were NO, NO_2, N_2O_5, HNO_3, N_2O and O_3 at the same time and place in the stratosphere for the full range of concentrations expected during a diurnal cycle. These trace gases play a key role in the present characteristics of the ozone layer. The prescribed measurements would improve our understanding of how aircraft engine emissions might affect the ozone layer and the stratosphere. The Hybrid Gas Conversion System was selected to make these measurements. As discussed in the Feasibility Study, the hybrid system consists of a UV absorption instrument for O_3, a gas chromatography instrument for N_2O, and a chemical conversion/chemiluminescent instrument for HNO_3, N_2O_5, NO_2, and NO. The expected sensitivity for O_3 is 2.7×10^{10} and for N_2O is 3.7×10^9 molecules/cm^3. The third instrument consisted of a thermal converter for the HNO_3 and N_2O_5 selective conversions, a photolytic or catalytic converter for the NO_2 selective conversion, and a chemiluminescent detector for the NO detection. The flow of stratospheric gas through the system would be operated on in appropriate sequences by these converters to measure each species in turn using the sensitivity detector. The expected sensitivity for NO is 1.3×10^7 molecules/cm^3 for a 1-sec integrating time. The expected sensitivity for the remaining species would be comparable. The accuracy for the remaining species, however depends on the specificity of the conversion techniques for each species in the presence of the others and in the presence of other possible nitrogen oxide species in the stratosphere (e.g. HO_2NO_2 and $ClONO_2$).

The Feasibility Study recommended development and deployment of the Hybrid Gas Conversion System and, simultaneously, a laboratory study of the specificity issues. This report documents the laboratory measurements made to resolve specificity and other issues. Particular emphasis was placed on (1) the conversion of NO_2 to NO by both catalytic and photolytic converters, (2) thermal conversion of N_2O_5 and HNO_3 to NO_2 with and without possible interfering gases, and (3) the feasibility of measuring total odd-nitrogen concentrations using catalytic thermal conversion (in conjunction with the NO and NO_2 measurements). The conversion of NO_2 to NO by catalytic techniques, if reliable, would mean a significant weight reduction in the balloon payload. In brief, the laboratory measurments consisted of breadboarding the various converters, testing

them with known concentrations of species, and generating as necessary those species which are highly reactive. The laboratory measurements were supported by computer modeling of the conversion process and the flow through the instrument. The modeling was then used to extrapolate the performance of the laboratory instrument to its expected performance in the stratosphere. A summary of the results of the laboratory measurements is given in Section II. Section III describes the measurements and their interpretation in detail. Conclusions and recommendations arising from this study are presented in Section IV.

SECTION II

SUMMARY

Extensive laboratory measurements for the detection and measurement of NO, NO_2, N_2O_5 and HNO_3 have been carried out for various types of chemical conversion instrumentation. Particular emphasis was placed on the conversion of NO_2 to NO by both catalytic and photolytic converters, thermal conversion of N_2O_5 and HNO_3 to NO_2 with and without possible interfering gases, and the feasibility of measuring total odd-nitrogen concentrations using catalytic thermal conversion. Computerized chemical kinetics simulations have also been generated to independently support the laboratory measurements and expected performance of instrumentation at stratospheric float altitudes.

For NO measurement, gas phase titration with O_3 is employed followed by the monitoring of the chemiluminescence of an excited state of NO_2 formed during the titration. This method is well understood, and possesses ample sensitivity to meet the HAPP requirement of 10^8 molecules/cm^3 at stratospheric altitudes.

Analytical methods for the remaining three species employed various techniques for quantitatively converting the molecule directly or indirectly to NO, followed by the chemiluminescent technique cited above.

For NO_2 conversion to NO, four techniques were utilized at a typical laboratory concentration of 1×10^{14} molecules/cm^3 and less. Three techniques employed some form of catalyst. The remaining technique was the photolytic conversion of NO_2 to NO using radiation the in 300-400 nm spectral region. The reactant, NO_2 was also monitored using a high temperature catalytic converter followed by chemiluminescence. The product, NO was monitored by the chemiluminescence technique. Photolytic converter efficiency has been determined to be as high as 57 percent and is a function of photon flux and sample residence time. Efficiency, therefore, is a design engineering tradeoff problem.

This technique was evaluated because specificity with other possible nitrogen oxide species of the stratosphere is not an issue. Of the catalytic conversion techniques evaluated, only the high temperature (800 K) catalytic conversion was found to be very efficient for NO_2 but, unfortunately, the technique cannot be used for NO_2 as N_2O_5 and HNO_3 would be simultaneously converted. Chemical-thermal conversion of NO_2, an adjunct to thermal-catalytic conversion, although not evaluated in the lab, was reviewed as a technique. Efficiency of conversion for this technique, however, has been found to be low when an oxidant such as ozone is present (Lowenstein, private communication, 1978). Catalytic-chemical conversion of NO_2 was evaluated as a technique using both ferrous sulphate, $FeSO_4$, and ferrous ammonium sulphate, $Fe(NH_4)_2$-$(SO_4)_2$. With $FeSO_4$ as a catalyst, not only was the conversion efficiency found to be low but also substantial quantities of NO_2 were lost, presumably by an adsorption process. This technique is known to be a poor converter of NO_2 when an oxidant (O_3) is present in the sample (Ridley and Schiff, 1978). With $Fe(NH_4)_2(SO_4)_2$ as catalyst, the conversion efficiency was found to be high (greater than 97.5 percent) once procedural problems associated with Viton* were eliminated. Catalytic-sorption converters, either platinum or platinum and palladium, on a support column were found to be ineffective for conversion of NO_2.

Thermal conversion of N_2O_5 to NO_2 at a typical laboratory concentration of 7×10^{13} molecules/cm^3 was found to be straightforward with the decomposition going to completion at a temperature of 475 K. Nitrogen pentoxide which cannot be stored at room temperature for any practical length of time was generated as needed in a kinetic flowing system. Product and reactant species number densities were monitored by IR absorption and, for NO_2 and NO, by catalytic-thermal conversion and chemiluminescence, respectively. The rate limiting reaction rate and stoichiometry were monitored a number of times and found to be in agreement with the other workers in the field.

*Viton is a trade name for the copolymer form of vinylindene fluoride and hexafluoropropylene.

Two procedural issues with N_2O_5 observed during the laboratory studies are related to the generation and decomposition of N_2O_5. First, if moisture is present on the walls of reaction vessels in use during the generation process, HNO_3 is formed and the N_2O_5 yield is less than unity. Although this is a heterogeneous reaction, the homogeneous formation or desorption of HNO_3 was also observed. This HNO_3 formation was employed for simultaneous species testing of thermal converters. Hence the issue was resolved and the artifacts used as an advantage. Second, for most tests carried out, high purity oxygen was employed for generating ozone so as to oxidize NO_2 to NO_3 and thus generate N_2O_5. For long term stable storage of NO_2, the diluent gas selected was high purity air. Upon reacting NO_2 and O_3, the resulting carrier gas was oxygen rich reaching at times 78 percent which is atypical of air. Thus it is conceivable that significant oxidizing reactions were occurring when the experimental objective was to carry out reducing reactions.

Thermal conversion of HNO_3 at a typical laboratory concentration of 2 x 10^{14} molecules/cm^3 to NO_2 and thermodynamically predicted NO was found to be straightforward with the decomposition going to completion at a temperature as low as 535 K. Product and reactant species number densities were monitored by IR absorption and, for NO_2 and NO, by catalytic-thermal conversion and chemiluminescence, respectively. The decomposition is not promoted by a catalyst but does require a surface presumably to scavenge the product OH radical. Computer analysis, (Appendix B), does confirm a faster decomposition rate when OH is scavenged from a stream operated at sea level conditions. Computer analysis for stratospheric conditions where there is a preponderance of O_3 indicates O_3 does not impact conversion, but also that complete conversion requires a temperature of about 800 K. Nitric acid decomposition tests in the presence of nitrogen, separately in the presence of air, and again separately in the presence of oxygen enriched air are presented. Nitric acid decomposition tests in the presence of relatively high levels of O_3 have also been carried out.

Potential interferents reviewed analytically or theoretically included chlorine nitrate, $ClONO_2$, and pernitric acid, HO_2NO_2. Both are considered

to be labile with the former undergoing conversion at 350 K and the later at about 300 K. If these species are actually present in the stratosphere at number densities greater than instrumentation detection levels, their presence reduces specificity of a particular thermal conversion.

The lack of specificity of thermal converters can actually be used to advantage for the detection of total odd nitrogen species, NO_z. Rather than be concerned about the possible presence of such species as $ClONO_2$ and HO_2NO_2 or about the partial decomposition of HNO_3 when N_2O_5 is being totally decomposed, all odd-nitrogen species in the stratosphere would be decomposed to NO using a high-temperature catalytic converter. This possibility was recommended in the Feasibility Study and its feasibility is shown here, based on the above measurements and on analytic modeling. The instrument would consist of two similar channels, an NO channel at 250 K and a total odd-nitrogen channel at 800 K.

One new technique under development for the measurement of NO_2 promises sensitive and specific measurements in a lighter and more compact module. Narrowband UV photolysis of NO_2 leaves NO in an excited state from which its characteristic fluorescence can be measured. Also, the technique could be extended to NO by first converting NO to NO_2 as is done in the chemiluminescent detector. The potential of the technique is critically assessed based on discussions with J. Anderson of Harvard and D. Kley of NOAA.

Finally, the analytic computer models of the conversion techniques developed to model the laboratory measurements have been used to assess the techniques under stratospheric conditions. The modeling results for both laboratory conditions and those for the stratosphere's expected concentrations indicate, with only minor differences, identical conversion trending. This permits valid extrapolation of the laboratory results. Thus, it is concluded that there is no fundamental reason why these techniques would not work at the required sensitivities in the stratosphere. However, sample fidelity and surface reactions which are not amenable to modeling must be given closer attention in laboratory conditions closer to those of the stratosphere.

SECTION III

PERFORMANCE TESTING AND EVALUATION

This section is devoted to theoretical considerations and laboratory measurements for various analytical methods for the detection of nitric oxide, nitrogen dioxide, nitrous pentoxide and nitric acid. Generation of the latter two gases at quantitative concentrations is also presented. The final three subsections are devoted to considerations of potential interferents, the feasibility of a total odd-nitrogen measurement, and the promise of a new technique for nitrogen dioxide, NO_2.

Each subsection presents the appropriate theoretical considerations followed by experimental findings.

As many chemical reactions are listed throughout this report, and their reaction rates evaluated, particular conventions and procedures are employed. Often recourse is made to chemical thermodynamic equilibrium constants. In the main, accepted conventions for notation have been used (Hampson and Garvin, 1978). For example, consider the reaction below with the forward reaction rate coefficient k_f,

$$A + 2B \rightarrow AB_2, \quad k_f,$$

$$\frac{d[A]}{dt} = \frac{1}{2}\frac{d[B]}{dt} = -\frac{d[AB_2]}{dt} = -k_f[A][B]^2,$$

where $[A]$ is the concentration of constituent A and so forth. Similarly, the backward reaction can be expressed with the reverse reaction rate coefficient k_r,

$$AB_2 \longrightarrow A + 2B, \quad k_r.$$

$$\frac{d[AB_2]}{dt} = -\frac{d[A]}{dt} = -\frac{1}{2}\frac{d[B]}{dt} = -k_r\,[AB_2].$$

At equilibrium, the total time derivatives vanish, leading to the equations

$$k_f [A] [B]^2 = k_r [AB_2] ;$$

$$K_e = k_f/k_r = \frac{[AB_2]}{[A] [B]^2} , \qquad (3\text{-}1)$$

where K_e is the equilibrium constant for this reaction expressed in units of concentration (usually moles/liter or molecules/cm^3). Usually, only one reaction rate coefficient is known so that an evaluation of K_e must be made in order to derive the opposing reaction rate coefficient. The primary source of information with respect to the equilibrium constant is the set of JANAF Thermochemical Tables. These tables list as a function of temperature the thermochemical properties of most of the compounds of interest in this report. These properties are related to the equilibrium constant by the following expression

$$-R \ln K_p = \Delta(G^\circ_T - H^\circ_{ref})/T + \Delta\left(H^\circ_{ref}/T\right) \qquad (3\text{-}2)$$

where K_p is the equilibrium constant in units of atmospheres (atm). Δ represents the sum over the products of the reaction minus the sum over the reactants. The quantity $(G^\circ_T - H^\circ_{ref})/T$ is known as the Gibbs-energy function. The subscript, ref, is the reference point temperature (298.15 K for these tables). ΔH°_{ref} is the heat of formation of the constituent at the reference temperature. The superscript symbol, °, signifies atmospheric pressure (760 torr). K_p can be related to K_e.

$$K_p = K_e (RT)^{\Delta n}$$

where Δn is the change in the number of moles of constituents (moles of products minus moles of reactants). Thus,

$$K_e = (RT)^{-\Delta n} \exp\left[-\frac{1}{R}\Delta\left(\frac{G^\circ_T - H^\circ_{ref}}{T}\right)\right] \exp\left[-\frac{1}{RT}\Delta\left(\Delta H^\circ_{ref}\right)\right] .$$

Typically, the Gibbs-energy function changes slowly over the temperature range of interest ($220\ K \leq T \leq 900\ K$). The principal temperature dependence is contained in the second exponential factor. For most reactions $\Delta n = 0$ or ± 1, so that the effect of temperature in the leading term in the expression is not pronounced. It proved convenient for computer coding to assume that the leading exponential term was independent of temperature.

As noted, usually only one reaction rate coefficient has been measured. A critical review of such coefficients for reactions among atmospheric constituents has been made by Hampson and Garvin (1978). Their recommended values have been used wherever possible in computer modeling codes. Other sources will be cited as required for any reactions not included in the review. If the opposing reaction rate coefficient has also been measured, then it is incorporated directly. Otherwise, the equilibrium constant is evaluated in the manner described above and the opposing reaction rate coefficient is derived, equation 3-2.

Reactions are numbered sequentially throughout the document. The equilibrium constant is denoted as $K_{number, -number}$. Forward reaction rate coefficients are denoted as k_{number} and reverse reaction rate coefficients as $k_{-number}$.

In some cases a laboratory or net stoichiometric reaction is presented and followed by a set of redox reactions or mechanism. As none of the authors are kineticists, Glasstone et al. (1941)-type graphical representations of the mechanism, e.g., potential energy, standard-state molal free energy or enthalpy versus reaction coordinate were considered to be qualitative or too symbolic for use in applying reaction rate theory.

3.1 NITRIC OXIDE CHEMILUMINESCENCE SENSOR

3.1.1 Theory

As a part of CIAP, stratospheric NO was measured by Ridley et al. (1972) using the chemiluminescent method, specifically the ozone oxidation of NO to an optically excited state of NO_2. The method is also being used by Dr.

Schmeltekopf's group at NOAA for stratospheric measurements and Dr. Stedman's group at NCAR for tropospheric measurements. The method is based upon the reactions:

$$NO + O_3 \longrightarrow NO_2^* \left({}^2B_1\right) + O_2 \qquad (1a)$$

$$\longrightarrow NO_2 \left({}^2A_1\right) + O_2 \qquad (1b)$$

$$NO_2^* \longrightarrow NO_2 + h\nu\ , \lambda \geq\ 600\ nm \qquad (2)$$

$$M + NO_2^* \longrightarrow M + NO_2,\ M = O_2 \text{ or } N_2 \qquad (3)$$

The bimolecular second order rate constants, k_{1a} and k_{1b}, are given by Clough and Thrush (1967) as:

$$k_{1a} = 7.6 + 1.5 \times 10^{11} \exp\ (-4180 + 300/RT)\ cm^3\text{-mole}^{-1}\text{-s}^{-1}$$

$$= 1.26 \times 10^{-12} \exp\ (-4180/RT)\ cm^3\text{-molecule}^{-1}\text{-s}^{-1}$$

and

$$k_{1b} = 4.3 + 1.0 \times 10^{11} \exp\ (-2330 + 150/RT)$$

$$= 7.13 \times 10^{-13} \exp\ (-2330/RT)$$

Since reaction (1a) has a higher activation energy, luminescence is favored if the temperature is as high as practical. At room temperature, 298 K, the rates k_{1a} and k_{1b} are 1.08×10^{-15} and 1.39×10^{-14} cm^3-molecule $^{-1}$-s^{-1}. Therefore, of the NO molecules that react with the O_3, only $k_{1a}/(k_{1a} + k_{1b})$ or 7.2 percent are converted to NO_2^*. These then radiate via reaction (2) or are quenched via reaction (3).

The intensity of the chemiluminescence (CL) emission is given by Clyne et al. (1964) as:

$$I = \frac{\left[I_o\right]\ NO\ \left[O_3\right]}{\left[M\right]} \qquad (3\text{-}3)$$

provided that $k_3 \left[M\right] >> k_2$ with $\left[M\right]$ denoting total pressure in molecules/ cm^3. The value of I_o is given approximately as 12 exp (-4180 ± 300/RT) photons/s

for the spectral region 650 to 875 nm (Fontijn et al., 1970). The broadband output serves to make this a non-specific method for NO, however, experience shows that daytime NO can be reliably measured. Clyne et al. (1964) report a less conservative value of 20.7 for the coefficient. At room temperature, 298 K, $I_o = 1.0 \times 10^{-2}$ photon/s and at 316 K, 1.54×10^{-2} photon/s. Since $k_2/k_3 = 2.7 \times 10^{14}$ molecules/cm^3, the above inequality is valid to pressures as low as 4.5 torr or an altitude of 35 km (Clough and Thrush, 1967).

Achieving linearity with the CL method requires that a negligible net amount of O_3 be consumed by the NO in a flowing system. The combined bimolecular second order reaction rate, k_1, is given by Johnston and Crosby (1954) as:

$$k_1 = 0.8 \times 10^{12} \exp(-2500/RT) \text{ cm}^3\text{-mole}^{-1}\text{-s}^{-1}$$
$$= 0.13 \times 10^{-11} \exp(-2500/RT) \text{ cm}^3\text{-molecule}^{-1}\text{-s}^{-1}$$

The rate constant is related to the concentrations through,

$$-\frac{d[O_3]}{dt} = -\frac{d[NO]}{dt} = k_1 [NO][O_3] \qquad (3\text{-}4)$$

Assuming that the second reactant gas concentration, $[O_3] >> [NO]$, the integrated second order rate law is:

$$\frac{1}{[O_3]} \ln \frac{[NO]}{[NO] - \Delta[NO]} = k_1 t = 0.19 \times 10^{-13} t \text{ at } 298 \text{ K} \qquad (3\text{-}5)$$

or

$$\frac{\Delta[NO]}{[NO]} = 1 - \exp\left(-[O_3]\,0.19 \times 10^{-13} t\right) \qquad (3\text{-}6)$$

If the exponent is made large (4 or 5), then the photomultiplier sensitivity (PMT current per unit NO mass flow rate) is proportional to

$$\left(\frac{k_{1a}}{k_{1a} + k_{1b}}\right) \frac{GQ_{NO}}{P}$$

where G denotes a geometric factor. In terms of reactor volume V, temperature T, reactant flow rate Q_{NO}, and second reactant flow rate Q_{O_3}, the quantity $[O_3]$ after mixing with the sample stream is for a constant volume sampling pump:

$$\left[O_3\right] = \left[O_3'\right] \frac{Q_{O_3}}{Q_{NO} + Q_{O_3}} \left(\frac{P}{760}\right) \left(\frac{273}{T}\right) \qquad (3\text{-}7)$$

where $\left[O_3'\right]$ denotes ozone concentration at the internal generator.

The exponent becomes:

$$\simeq 0.19 \times 10^{-13} \left[O_3'\right] V \left(\frac{Q_{O_3}}{Q_{NO}^{\,2}}\right) \left(\frac{P}{760}\right)^2 \left(\frac{273}{298}\right)^2$$

Silent discharge O_3 generators can produce as much as 3 percent ozone at a flow rate of 25 scc/s. Using these values and reasonable values for volume and sample flow rate yields:

$\left[O_3'\right]$ = 3% so that $\left[O_3'\right] = 8.07 \times 10^{17}$ molecules/cm^3

$V = 1.0 \times 10^3$ cm^3

Q_{O_3} = 25 scc/s

$Q_{NO} = 2.5 \times 10^2$ scc/s

The exponent and relative extent of the reaction taking place within the reactor can be indicated as a function of altitude, as presented below in Table 3-1. Significant departures from a 100 percent extent of reaction can lead to non-linearities and measurement errors.

TABLE 3-1. $\left[O_3\right] k_1 t$ TERM VS ALTITUDE FOR ABOVE VALUES

Altitude, H (km)	Pressure (torr)	$\left[O_3\right] k_1 t$	$\Delta\left[NO\right]/\left[NO\right]$
15	99.0	54.8	1.00
25	21.3	5.9	1.00
35	4.9	86.8	0.934
		4.15	1.00
		0.22	0.98
			0.20

For the parameters selected above, the CL method would be limited to a maximum altitude of about 25 Km. Increased reaction volume, 50 percent, and ozone flow rate, 100 percent, could extend the altitude limit to about 30 Km.

3.1.2 Experimental Procedures and Results

An Aerochem AAS-3S chemiluminescence monitor was extensively employed for general purpose and process control mmasurements of NO. By reversing the role of the second reactant gas, in this case O_3, ozone could also be monitored. The commercial specifications for this instrument are presented below in Table 3-2.

TABLE 3-2. AEROCHEM RESEARCH AAS-3S SPECIFICATIONS

Useful range	0.1 to 10,000 ppb
Scales	Seven full scales 10, 25, 100, 250, 1000, 2500 and 10,,00 ppb
Accuracy	Limited by calibration sample
Linearity	±1% oo full scale
Interferences	NH_3 in NO_x mode
Time Response	11 sec on all scales
Time to Switch from One Gas to Another	Less than 15 seconds
Zero Drift	±2% in 24 hours
Gas Flow Rates	Sample ≈ 2.1 l(STP)min^{-1} Air/O_3 ≈ 0.4 l(STP)min^{-1}
Normal Temperature Range	15-35°C (59-95°F)
Normal Line Voltage Range	105125 volts
Electronics	Six inch analog meter on front panel with adjustable recorder output of 0 to 1 volt on rear panel.

Calibration of this type of instrument is based upon round-robin intercomparisons of several instruments and several calibration samples. Field collaborative testing of the chemiluminescence procedure is discussed by Paul C. Constant Jr. et al. (1975).

Design details for the Aerochem monitor, as well as those for the original B.A. Ridley et al. (1972) NO sensor, are given in Table 3-3. Although there are significant design differences between the instruments, the basic detection and measurement of NO is the same. The design differences are related primarily to the internal ambient pressures, reaction volumes, and flow rates and secondarily to the mode of operation used for the photomultiplier tube. The PMT is operated in an analog mode for the laboratory unit whereas for the stratospheric unit it is in a photon counting mode.

Two numerical examples are included in the table for each instrument. For the laboratory unit, an NO mixing ratio of 1 ppb(v) is assumed. For equation 3-3, this yields an intensity of $3 \times 10^5 h\nu/cm^3$-s. At the anode of the PMT the signal level is given by:

$$S_a = IV_R eG(Q.E.) \qquad (3\text{-}8)$$

where V_R denotes reaction volume. For the above example, assuming a 10 percent effective quantum efficiency, there is a 3×10^{-7} amp signal level. For the stated anode dark current a noise equivalent detection limit of 7×10^{-3} ppb can easily be derived. For the stratospheric unit, an NO mixing ratio of 4 ppb(v) was adopted. For a reaction temperature of 300 K, equation 3-3 yields an intensity of about $1.9 \times 10^4 h\nu/cm^3$-s. Since a mixing ratio of 4 ppb yields a signal level of 1.7×10^3 counts/s, the effective emitting volume-quantum efficiency product of 0.088 cm^3 is obtained. Assuming an effective quantum efficiency of 5 percent, an effective emitting volume of about 1.8 cm^3 is obtained, which is considerably less than the actual reaction volume.

With stratospheric instrumentation, a lowest detection limit of 5×10^7 molecules/cm^3 has been verified (B.A. Ridley et al., 1972).

TABLE 3-3. DESIGN COMPARISON OF NO CHEMILUMINESCENCE SENSORS

Developer Type	Aerochem Research Lab (1977) Laboratory Monitor	B.A. Ridley et al., (1972) Stratospheric Research
Operating Pressure	250 torr	33 torr
Sample Flow Rate	35 scc/s	210 scc/s
Reactant Flow Rate	6.7 scc/s	10 scc/s
Reaction Volume, V_R	10 cm^3	400 cm^3
Reaction Temperature	316 K	≃300 K
Residence Time	0.07 s	1.9 s
Detector	Centronics 4283 RA	EMI 9558 QA[b]
Temperature	5°C	-20°C
Gain	$6x10^6$	$3x10^7$
Dark Current	2.0 nA	85 cts/s
Conversion Factor[a]	$9.76x10^{-13}cm^3$-coul	$8.9x10^{-2}cm^3$
NO Mixing Ratio	1 ppb(v)	4 ppb(v) at 33 torr
NO	$9.64x10^9$ molecules/cm^3	$4.25x10^9$ molecules/cm^3
O_3	$1.97x10^{16}$	$4.83x10^{14}$
M	$7.64x10^{18}$	$1.06x10^{18}$
$I_o[NO][O_3]/[M]$	$3.0x10^5 h\nu/cm^3$-s	$1.94x10^4 h\nu/cm^3$-s
Signal	$3.0x10^{-7}$A	$1.7x10^3$cts/s
Responsivity	300 nA/ppb	10^{-1} nA/ppb (360 cts/ppb)
Noise Equivalent Detection Limit	0.007	0.05 ppb
Lowest Detection Limit	0.1 ppb	0.05 ppb
Linearity	$0.1-10^4$ ppb (1%)	0.05-34 ppb

[a] Conversion factor = $V_R eG(Q.E.)$.

[b] An RCA 31034A photomultiplier was used on the first flight yielding a responsivity of 1855 cts/ppb and a lowest detection limit of 0.02 ppb at an altitude of 22 Km or about 50 torr (Ridley et al., 1974).

3.2 NITROGEN DIOXIDE PHOTOLYTIC CONVERSION

Measurement of stratospheric NO_2 can take place by photolyzing the NO_2 to nitric oxide, followed by gas phase titration with O_3. This method has been developed and is being used by the NOAA group (MacFarland et al., private communication, 1977). This technique was evaluated because specificity with other possible nitrogen oxide species of the stratosphere is not an issue.

3.2.1 Theory

The mechanism for the photolytic conversion of NO_2 to NO and ground state atomic oxygen is at least a four step process; namely:

$$NO_2 + h\nu \longrightarrow NO + O(^3P) \quad \lambda \geq 300\text{nm} \tag{4}$$

$$O + NO_2 + M \longrightarrow NO_3 + M \tag{5}$$

$$O + NO_2 \longrightarrow NO + O_2 \tag{6}$$

$$NO + NO_3 \longrightarrow 2NO_2 \tag{7}$$

The above reaction set is a subset of the set employed by Stedman and Niki (1973) to account for the kinetics and mechanism for the photolysis of NO_2 in air. The expanded set includes O_3, NO_3 and N_2O_5 reactions. If only reactions 4, 5 and 7 are considered, the net quantum yield is zero. If only reactions 4 and 6 are considered, the net quantum yield is two. The actual yield lies between these values.

For the above set, the rate of change of NO_2 is given by:

$$-\frac{d\left[NO_2\right]}{dt} = k_4 \left[NO_2\right] + k_5 \left[O\right] \left[NO_2\right] \left[M\right] + k_6 \left[O\right] \left[NO_2\right] - 2k_7 \left[NO\right] \left[NO_3\right] \tag{3-9}$$

Since NO_3 will have a rapidly defined (microseconds) stationary value, i.e., $d\left[NO_3\right]/dt = 0$, the equation

$$k_5 \left[O\right] \left[NO_2\right] \left[M\right] = k_7 \left[NO_3\right] \left[NO\right] \tag{3-10}$$

can be used to simplify equation 3-9 to

$$-\frac{d[NO_2]}{dt} = k_4 [NO_2] - k_5 [O] [NO_2] [M] + k_6 [O] [NO_2] \text{ or} \qquad (3\text{-}11)$$

$$\frac{d\ln [NO_2]}{dt} = \frac{2k_1 k_6}{k_6 + k_5 [M]}$$

Equation 3-11 is often simplified to a first order dissociation. Examining the validity of this statement, one notes that $k_5 = 1.0 \times 10^{-31} cm^6\text{-molecule}^{-2}\text{-s}^{-1}$ and $k_6 = 9.2 \times 10^{-12}\ cm^3\text{-molecule}^{-1}\text{-s}^{-1}$ (Hampson and Garvin, 1978). At 1 atmosphere $M = 2.446 \times 10^{19}$ molecules/cm^3, so that $k_5 [M] = 2.446 \times 10^{-12}$ $cm^{-3}\text{-molecule}^{-1}\text{-s}^{-1}$ or about one-fourth that of k_6. For $k_4 < 0.75\ k_6 [O]$, the simplification is valid and the integrated form of equation 3-11 becomes:

$$\frac{[NO]_t}{[NO_2]_o} = 1\text{-exp } (-I\ \sigma t) \qquad (3\text{-}12)$$

$$\Sigma\ I(\lambda)\ \sigma\ (\lambda)\ d\lambda \qquad (3\text{-}13)$$

where $I(\lambda)$ corresponds to the photon flux rate and $\sigma(\lambda)$ the absorption cross-section. This expression assumes a quantum yield of unity for the dissociation, a valid assumption for $244 \leq \lambda \leq 398$ nm (Hampson and Garvin, 1973). The cross-section data of Johnston and Graham (1974) and that of NASA Publication 1010 (1977) have been used to obtain a value of k_4.

Since the conversion efficiency is dependent upon k_4 and sample residence time, t, it is important to maximize their product.

When O_2 is present in the sample stream, the above analysis is inadequate to predict experimental results. Two additional reactions impairing conversion efficiency are:

$$O + O_2 + M \longrightarrow O_3 + M \qquad (8)$$

$$NO + O_3 \longrightarrow NO_2 + O_2 \qquad (1)$$

when significant amounts of O_3 and NO are formed, reaction (1) inhibits the photolytic dissociation process.

The converter design selected used 1 kw a mercury capillary lamp (Illumination Industries, Inc. type AH6-1BC) in conjunction with Corning 7-54 and Pyrex filters to restrict the photon flux to a spectral region defined by approximately 300-400 nm. The photolytic rate for a unit area of radiation is given by

$$k_4A = \frac{10^7}{hc} \int_{280}^{420} \tau\lambda \ (P/\Delta\lambda) \ \sigma\lambda \ d\lambda \ cm^2\text{-}s^{-1} \qquad (3\text{-}14)$$

where

λ	denotes wavelength in cm
h	equals Planck's constant = 6.62×10^{-27} erg-s
c	equals the velocity of light = 3×10^{10} cm/s
10^7	denotes conversion factor for joules to ergs
τ_λ	denotes spectral transmittance of the optical filters
$P/\Delta\lambda$	denotes total radiated watts per 10 nm increments
σ_λ	denotes NO_2 absorption cross-section in cm^2/molecule, and
$d\lambda$	denotes variable of integration

With a new lamp operating at 1 kw and with the filters indicated, evaluation of the above expression yields $k_4A = 74\ cm^2\text{-}s^{-1}$ and $k_4 = 0.26\ s^{-1}$ for this design. The residence time for this cell is approximately 5 seconds so that the conversion efficiency is predicted to be 73 percent. The actual design and measured results for the photolysis of NO_2 is treated in the next two paragraphs.

3.2.2 Stratospheric-Based Instrumentation Modeling

Computer modeling predictions for stratospheric pressure are considered. For the case where P = 19 torr (25km), $k_5\ [M]$ is reduced by a factor of 40 and the photolytic conversion efficiency increases from 12.8 percent to 44 percent for $k_4 = 0.26\ s^{-1}$. Thus the performance of the photolytic technique improves with reduced pressure.

3.2.3 NO_2 Photolytic Converter Design

Prior to discussing the procedures and results for the NO_2 photolytic converter, the design of the laboratory converter is presented. The design

of the overall converter was based upon the availability of a photochemical lamp, expedience of attaining the proper spectral filtering and material chemistry aspects.

The high pressure mercury arc capillary lamp is of the straight bore type with a rating of 1 kva. The lamp, part number AH6-1BC, was obtained from Illumination Industries, Inc. To dissipate non-radiative heat, a water cooling jacket was provided. The jacket comprises two concentric cylinders made of quartz and Pyrex. The Pyrex was selected to attenuate radiation below about 300 nm. To suppress radiation above about 400 nm, Corning filter glass 7-54 was employed and configured as a hexagonal cylinder circumscribing the outer cooling jacket. The filter glass elements were held in place by teflon disks supported inside a gold-plated aluminum cylinder which served as the photolytic reaction vessel.

Lamp cooling with high pressure Hg lamps is critical and one is constrained to maintaining the temperature over a finite range so that the proper vapor pressure of mercury is attained while simultaneously minimizing stresses in the quartz envelope. Also steam must be prevented from forming on the quartz envelope. To achieve the above requirements the lamp is used in a horizontal position, chilled de-ionized water is flowed through the water jacket assembly at a rate of 1-1.5 gpm, and an inner jacket or "velocity tube" is employed to minimize the water volume near the lamp envelope, thus increasing the flow velocity.

An a-c power supply, employed for driving the lamp, consists of a line voltage variac, 4 kva transformer, current monitor and voltage monitor. The transformer of a soft iron design has built-in leakage inductance. To assist in starting the lamp at a reasonable voltage close to operating voltage, a small amount of argon is contained within the lamp envelope. The voltage waveform is typically a square wave with a slight overshoot on the leading edge.

Design parameters for the photolytic cell are given in Table 3-4.

TABLE 3-4. NO_2 PHOTOLYTIC CELL DESIGN

Parameter	Value
Lamp Luminous Length	2.54 cm
Lamp Bore Diameter	0.2 cm
Quartz Velocity Tube ID, OD	12, 15 mm
Pyrex Tube ID, OD	36, 41 mm
Corning Filter Facet Width	2.2 cm
Sample Cylinder ID	10.3 cm
Effective Radiative Area	280 cm^2
Radiated Sample Volume	177 cm^3
Sample Flow Rate	2.1 SLPM
Sample Residence Time	5.05 s
Lamp Current	1.2 amps
Lamp Voltage	435-700 V
Lamp Power	552-840 W
Near UV (320-400 nm) Radiated Power	112.3 w @ 1 kva
365 nm Radiated Spectral Power	3.6 w/nm
Radiated Power/Input Power	0.46
Materials Exposed to NO_2 Sample	Gold, stainless steel 303, Teflon, Corning glass, Pyrex
NO_2 Design Conversion Efficiency @ 1 kva	73 percent

3.2.4 Experimental Procedures and Results

Pre-mixed and calibrated samples of NO_2/air were obtained from Airco in aluminum Spectra-Seal® cylinders. Airco calibrations of 0.6-10 ppm concentrations were verified using the catalytic thermal converter of the Aerochem CL monitor discussed in paragraph 3.1.

Sample pressure was reduced and regulated using Matheson type regulators containing stainless steel diaphragms. Sample flow rate was set by the Aerochem CL monitor pump and internal sonic orifice. All other plumbing was either stainless steel or teflon® (PTFE)*.

*PTFE, polytetrafluorethylene

Relatively new lamps (less than 10 hours of aging) were employed; however no effort was expended in logging the number of on-off cycles which do affect lamp life. In operation the cell was connected in series with the CL monitor. With the Hg lamp in the off state, the CL monitor was set to the NO_x mode to measure the NO_2 entering the photolytic cell. The lamp was then excited and the CL monitor was placed in the NO mode to measure the amount of NO leaving the photolytic cell. If there was no or negligible NO in the supply gas then the ratio of the two measurements was simply the converter efficiency.

The results of the tests are given in Table 3-5 for various lamp power levels. Assuming a linear relation between input power and radiated power, the various anticipated rates and converter efficiencies are included. The measured efficiencies do not correspond directly to the calculated efficiencies but this is expected, since the rates were derived from brochure data and not measured values. The computer derived efficiencies are in large variance with the measured efficiencies. An attempt to account for this variance is given below.

TABLE 3-5. CALCULATED AND MEASURED NO_2 PHOTOLYTIC CONVERTER EFFICIENCIES

Lamp Voltage (Volts)	Lamp Power (Watts)	k_4 (s^{-1})	First Order Calculated Efficiency (Percent)	Computer Code $\Delta[NO]/\Delta[NO_2]$	Measured Efficiency (Percent)
435	522	0.14	50	0.58	35
525	630	0.17	57	0.64	45
700	840	0.22	67	0.63	57
-	1000	0.26	73	0.62	-

The oxidation of NO_2 by $O(^3P)$ has a predominating effect for producing the intermediary, NO_3 with k_5 M being 2.36×10^{-12} cm^3/molecule-s. The NO_3 is then available to react with NO_2 forming N_2O_5, or with NO forming NO_2. Formation of NO_2, reaction (7), proceeds at a rate about an order of magnitude faster than the formation of N_2O_5. Thus, as previously mentioned, the quantum

yield is reduced. If the ground state oxygen atom were scavenged by some other means, then the predicted yield would increase.

From this data one notes that efficiency is a design engineering trade relating power with photon flux as well as sample residence time. The residence time is of course related to the selected photolytic cell volume and the flow selected for the high sensitivity NO chemiluminescence monitor.

3.3 NITROGEN DIOXIDE CATALYTIC CONVERSION

Results obtained in employing several types of catalytic converters for NO_2 measurements are reported in this section. The types included are (1) catalytic-thermal converters, (2) chemical-thermal converters, (3) catalytic-chemical converters and (4) catalytic-sorption converters.

Significantly different results have been found for type (1) and type (2) converters when O_3 is present. A type (1) converter used in this study employs a noble metal while the type (2) converters investigated by Dr. Max Lowenstein of NASA employed a metal readily oxidizeable. Section 3.3.1.1 attempts to justify the widely disparate results observed with these converters.

3.3.1 Catalytic/Chemical Thermal Converters

3.3.1.1 Theory

Since much of the data reported upon in subsequent sections is based upon catalytic thermal conversion, a review of thermal converters both catalytic and chemical is warranted.

Table 3-6 lists various metals and carbon which have been used in NO_x or NO_2 converters. The listing has been arranged in decreasing value of the Gibbs or free energy formation of the oxide of the metal (or carbon). If the free energy value listed is negative, the reaction can occur. The reverse reaction, decomposition, would then have a positive value and would not occur. The last column corresponds to the mininum temperature required to achieve about 98 percent conversion of NO_2 for non-oxidized surfaces (L.P. Breitenbach and M. Shelef, 1973).

TABLE 3-6. FREE ENERGY OF FORMATION Δ F' (kcal/OXYGEN ATOM) AND TEMPERATURE FOR 98 PERCENT NO_2 CONVERSION

		300 K	400 K	500 K	T(°C)
Unstable Oxide	X[a]				600-1000
	Ag			+ 0.06	
	C	-32.8	-35.0	-37.1	400-600
	Ni			-46.1	750[b]
	Fe	-59.2	-57.1	-54.9	725-750[c]
	Mo	-63.6	-61.4	-59.3	525
	W	-63.7	-61.5	-59.3	475
	Mn			-83.1	475
Stable Oxide	V			-89.0	475

(a) Other noble metals
(b) Inconel; 80% Ni, 14% Cr, 6% Fe
(c) Monel; Stainless steel 304 and 316

As noble metal oxides have positive energies of formation, they are unstable and do not readily form in the presence of oxidants. Generally, they act as catalysts for many oxidizing and reducing reactions. In the case of NO_2 conversion, their inertness quality must be traded off against minimum conversion temperature.

For the remaining elements, NO_2 conversion proceeds according to the reactions:

$$NO_2 \rightleftharpoons NO + 1/2\ O_2 \tag{9}$$

$$M + O_2 \rightarrow MO_2,\ M = (Mo, W, Mn, V) \tag{10}$$

With increased usage, i.e. surface oxidation, the conversion temperature must be increased to effect the same conversion efficiency.

For the elements with negative free energies of formation, the element acts as an oxygen scavenger. As the free energy of formation becomes more

negative, the conversion temperature can be reduced since the oxidation becomes more preferred. For any given metal, as the temperature is increased, the free energy of oxide formation is shifted toward more positive values, thus reducing its effectiveness for NO_2 reduction. The use of carbon, coke in metallurgical ore reduction, permits lower temperature operation and the conversion proceeds as:

$$NO_2 + C \rightarrow NO + CO \tag{11}$$

As C is converted to CO or CO_2 in reducing NO_2 or by virtue of the oxygen molecules in an air stream, the surface material, C or M, becomes ineffective.

If a strong oxidant, O_3, H_2O_2, HNO_3, or HNO_4, is present in the sample stream, the surface material, C or M, is rendered ineffective at a faster rate.

From the above discussion, two facts are evident for NO_x converters. First, thermal converters employing true catalysts, e.g. platinum, stainless steel, and possibly nickel alloys, should be identified as catalytic-thermal converters, whereas the others (eg. Mo) should be identified as chemical-thermal converters. Second, chemical-thermal converters as defined above, can be expected to lose their efficiency if strong oxidants at significant concentration levels are present in the sample. The term "poisoning" is sometimes used to describe this efficiency loss but the definition is loose. Finally, to maintain efficiency, oxidant scavengers or scrubbers are often considered.

In the absence of any catalytic material, thermal conversion of NO_2 can also occur (Altshuller, 1957 and Breitenbach, 1973). The reaction, (9), is well understood and has been used to set converter temperatures. For oxygen at 152 torr, the ratio of $[NO_2]$ to $[NO]$ is given by:

$$\log \frac{[NO_2]}{[NO]} = \frac{3002}{T} - 4.2226 \tag{3-15}$$

3.3.1.2 Experimental Procedures and Results: Chemical-Thermal Converters

Experimental work by Dr. Max Lowenstein of NASA-ARC (private communication, 1978) has shown that for medium temperature molybdenum-based converter construction, NO_2 conversion may drop to zero if O_3 is present in the sample stream. It is felt that a two-body chemical reaction plus surface chemistry may be occurring.

The following two-body mechanism may also be occurring as an abnormal situation. First,

$$NO_2 + O_3 \rightarrow NO_3 + O_2 \qquad (12)$$

which is very fast, a factor of 50 due to the high temperature, when compared to a 298 K temperature rate. The mechanism continues as follows:

$$NO_2 + NO_3 \rightleftharpoons N_2O_5 \qquad (13)$$

$$NO + NO_3 \rightarrow 2NO_2 \qquad (7)$$

with a net result of

$$NO + N_2O_5 \rightarrow 3NO_2 \qquad (14)$$

and also

$$2NO + O_2 \leftarrow 2NO_2. \qquad (15)$$

This last reaction is of the third order type and extremely slow with a rate constant

$$k_{15} = 3.3 \times 10^{-39}\exp(-1050/RT)\ \text{cm}^3\text{-molecule}^{-2}\text{-s}^{-1}.$$

3.3.1.3 Experimental Procedures and Results: Catalytic-Thermal Converters

The commercial converter in use at Perkin-Elmer is constructed of inconel, alumina and a 90% Pt-10% Rh wire heating filament. As such, it approximates an catalytic-thermal converter. Conversion efficiency of this unit, without O_3 present, was first determined by the accepted Federal Register (1973) method, which is based upon reaction (15) given above and the fast reaction ($k_1 = 1.66 \times 10^{-14}$ cm^3/molecule-s);

$$NO + O_3 \rightarrow NO_2 + O_2, \qquad (1)$$

both of which produce stoichiometric quantities of NO_2. For all tests with the converter at its design temperature of 1100°C, conversion was greater than 99.7 percent.

The next set of conversion determinations for the commercial unit were made with about 9 ppm O_3 present and 9.5 ppm NO_2. The average conversion efficiency was found to be 97.9 percent or about 1.8 percent less, which is in concurrence with findings at NASA-ARC but not of real significance.

Generation of NO from $O(^3P)$, a product of O_3 thermal decomposition, is a possibility if surface recombination of atmoic oxygen does not occur on the platinum surface. A brief series of tests was carried out to assure that the surface recombination mechanism was in fact sufficient to scavenge $O(^3P)$. The catalytic thermal converter of the Aerochem CL monitor was used at reduced temperature, approximately 750 K, and a stream of ozonized air was passed over the platinum-rhodium heating filament. The ozone concentration level was typically 2.7×10^{13} molecules/cm^3 (1.1 ppm). Measurement of NO_x downstream from the converter was typically 2.45×10^{10} molecules/cm^3 (1.0 ppb) greater than the measured (NO_x) upstream of the converter. During these tests, the trace contamination NO level of the air source was 1.6×10^{11} molecules/cm^3 (6.5 ppb), while the instrument noise level was 2.45×10^9 molecules/cm^3 (0.1 ppb). Summarizing this test data one may conclude that 99.9 percent of the $O(^3P)$ atoms recombined, thereby providing effective scavenging.

It is important to note here that (1) catalytic thermal conversion is more effective for reducing NO_2 to NO than thermodynamic conversion and (2) that large relative levels of O_3 do not seriously impact the conversion process.

3.3.2 Catalytic-Chemical Converters

3.3.2.1 Theory

For this type of converter ferrous sulphate and ferrous ammonium sulphate were employed.

Although the gas-solid phase chemistry is not well known for the action of NO_2 and $FeSO_4$, the appropriate acidic solution is well known. Fe^{++} reduces HNO_2 to NO, which in turn combines with Fe^{++} to form $Fe(NO)^{++}$. This ion has a characteristic dark brown color. If NO_3 is present, in the absence of the NO_2, reduction occurs, forming as before $Fe(NO)^{++}$. This latter reaction occurs only when H^+ are prevalent and temperature is relatively higher. These conditions occur at the liquid-liquid boundary layer, and a brown ring forms.

Ferrous ammonium sulphate is the better converter choice since it is known that $FeSO_4$ selectively removes oxidants, specifically ozone (Miller et al., 1971). The Ridley-Schiff group also confirmed this fact in early 1978 when employing $FeSO_4 \cdot 7H_2O$ to convert ppb levels of NO_2 when ppm levels of O_3 were present.

3.3.2.2 Experimental Procedures and Results

Tubular flow converters were constructed with glass, quartz wool packing and stainless steel fittings along with the dehydrated form of the sulphate.

The initial converters were sized to yield a space velocity (flow rate/catalyst volume) of about 93 min^{-1} and a superficial linear velocity (flow rate/converter cross-sectional area) of about 2.4×10^3 cm/min. The final converter used extensively with $Fe(NH_4)_2(SO_4)_2$ was designed to yield a space velocity of about 17.5 min^{-1} and superficial linear velocity of about 5×10^2 cm/min.

Initial tests (1 through 3) for each catalyst resulted in large percentage losses of the NO_2 as presented in Tables 3-7 and 3-8. Subsequent testing indicated that viton seals were acting as adsorbents. Particular emphasis was placed upon $Fe(NH_4)_2$ $(SO_4)_2$ since $FeSO_4$ is a selective remover of O_3. Procedural changes resulted in no detectable NO_2 loss for the subsequent $Fe(NH_4)_2$-$(SO_4)_2$ tests. Conversions were found to be consistently greater than 97.5 percent.

The use of $Fe(NH_4)_2$ $(SO_4)_2$ is a competitive technique to NO_2 300-400 nm photoylsis, however, careful packaging design of the catalyst bed is required

TABLE 3-7. FERROUS SULPHATE CATALYTIC CONVERTER TEST RESULTS

Test	Species	1	2	3
Pre-converter concentration	NO_x	4.2ppm	68ppb	68ppb
	NO_2	2.4	62	62
	NO	1.8	6	6
Post-converter concentration	NO_x	3.6	33.5	30
	NO_2	0	19.8	17.5
	NO	3.6	13.7	12.5
NO_2 converted	Δ NO	1.8	7.7	6.5
NO_2 unconverted		0.0	19.8	17.5
NO_2 entrapped	Δ NO_x	0.6	34.5	38.0
NO_2 % conversion		75	12.4	10.5
NO_2 % unconverted		0	31.9	28.2
NO_2 % entrapped		25	55.6	61.3

so as not to reduce sample flow rate significantly nor represent a significant pressure drop.

3.3.3 Catalytic Sorption Converters

For this series of tests, Matthey-Bishop catalysts, 1% Pt and 0.4% Pd with 0.1% Pt on support columns, were contained in glass tubing. The combined weight of the pellets was about 5 gms. Nitric oxide was reacted with O_3 to provide NO, NO_2 and a minimal amount of O_3. The resulting concentrations at the converter input are shown below for two tests using the 1% Pt catalyst.

	Test 1	Test 2
NO	3.15 ppm	5.20 ppm
NO_2	2.65	2.95
NO_x	5.8	8.15
O_3	5.5 ppb	0.5 ppb

TABLE 3-8. FERROUS AMMONIUM SULPHATE CATALYTIC CONVERTER TEST RESULTS

Test[a]	Species	1 (ppb)	2 (ppb)	3 (ppb)	4 (ppm)	5 (ppm)	6 (ppm)	7 (ppm)	8 (ppm)	9 (ppm)
Pre-converter concentration	NO_x	437	437	443	2.68	4.40	7.20	4.65	2.74	1.55
	NO_2	435	435	429	2.68	4.40	7.20	4.65	2.74	1.55
	NO	2	2	14	0.0	0.0	0.0	0.0	0.0	0.0
Post-converter concentration	NO_x	100	80	95	2.68	4.40	7.20	4.65	2.74	1.55
	NO_2	70	30	47	0.06	0.09	0.09	0.015	0.04	0.03
	NO	30	50	48	2.62	4.31	7.11	4.50	2.70	1.52
NO_2 converted	NO	28	48	34	2.62	4.31	7.11	4.50	2.70	1.52
NO_2 unconverted		70	30	47	0.06	0.09	0.09	0.15	0.04	0.03
NO_2 Entrapped	NO_x	337	357	348	0.0	0.0	0.0	0.0	0.0	0.0
NO_2 % conversion		6.44	11.0	7.9	97.8	97.9	98.7	96.8	98.5	98.1
NO_2 % unconverted		16.1	6.9	10.9	2.2	2.1	1.3	3.2	1.5	1.9
NO_2 % entrapped		77.5	82.0	81.1	0.0	0.0	0.0	0.0	0.0	0.0

(a) Tests 1 through 3 employed a converter with a space velocity of about 93 min^{-1} and a superficial linear velocity of about 2.4×10^3 cm/min. Tests 4 through 9 employed a converter with a space velocity of about 17.5 min^{-1} and a superficial linear velocity of about 5×10^2 cm/min. Tests 1 through 3 were conducted with viton seals which caused substantial absorption.

The NO, NO_x concentrations at the output of the converter were found to be equal to each other and equal to 1.42 and 2.80 ppm, respectively. From this data it was concluded that (1) NO_2 either converted, or was adsorbed or both, (2) a portion of the NO was adsorbed, and (3) from this data, it may be concluded that these materials are not considered to be useful. In light of these results, further planned tests were abandoned.

3.4 NITROUS PENTOXIDE (N_2O_5) GENERATION

As nitrous pentoxide (N_2O_5) is reactive and unstable in the gaseous state, it was generated as needed. For N_2O_5 synthesis, excess NO_2 or excess O_3 and the other reactant were mixed in an elementary type flow system. The reactant product NO_3 and NO_2 combined yielding N_2O_5. This technique approximates the approach used by others.

Process control and determination of initial concentration levels, i.e., before dynamic dilution, were carried out by IR absorption techniques. Measured concentration levels as opposed to predicted levels were desired because of the reactive nature of the particular species. The levels after dilution were then employed in the overall assessment of an appropriate chemical converter ahead of a chemiluminescent monitor. The specific details of the IR measurements are discussed in Appendix A.

3.4.1 Theory

Generation of gas phase N_2O_5 is best carried out by the ozone oxidation of NO_2 as it is reasonably stable in the presence of ozone. The governing reactions are:

$$NO_2 + O_3 \longrightarrow NO_3 + O_2 \text{ (rate determining)} \quad (12)$$

$$NO_2 + NO_3 \longrightarrow N_2O_5 \text{ and} \quad (13)$$

$$N_2O_5 \longrightarrow NO_2 + NO_3 \quad (-13)$$

where the equilibrium constant, $K = 1.2 \times 10^{-11}$ molecules/cm^3 at a temperature of 300 K. The reaction can be carried out with either $\left[NO_2\right]$ or $\left[O_3\right]$ in excess. Reaction (12) is about 34 kcal/mole exothermic. Measured stoichiometry $\left[\Delta NO_2/\Delta O_3\right]$ values are 1.88 and 1.68 for excess O_3 and NO_2, respectively (Wu et al., 1973), and 1.89 ±0.08 (standard deviation) (Graham, 1975).

Various experimental rate constant values for k_{12} are shown as an Arrhenius plot in Figure 3-1. The Arrhenius parameters for the results of Johnston and Yost (1949) are

$$k_{12} = 9.82 \times 10^{-12} \exp(-7000/RT)\ \mathrm{cm^3\text{-}molecule^{-1}\text{-}s^{-1}}$$

and for the results of Graham (1975) are

$$k_{12} = (1.34 + 0.11) \times 10^{-13} \exp(-4900 \pm 60/RT)\ \mathrm{cm^3\text{-}molecule^{-1}\text{-}s^{-1}}$$

where the uncertainties are standard deviation.

For design purposes an average value of $5.37 + 1.76 \times 10^{-17}$ $\mathrm{cm^3\text{-}molecule^{-1}\text{-}s^{-1}}$ ($1.32 + 0.43 \times 10^{-3}$ $\mathrm{ppm^{-1}s^{-1}}$) at 298 K and 760 torr was chosen.

The integrated rate equation for the bimolecular reaction is given by:

$$\frac{1}{[NO_2]_o - [O_3]_o} \ln \frac{[O_3]_o\left([NO_2]_o - [NO_3]\right)}{[NO_2]_o\left([O_3]_o - [NO_3]\right)} = k_{12} t \ (\mathrm{conc})^{-1} \qquad (3\text{-}16)$$

where the subscript denotes original concentration levels. This expression is plotted in Figure 3-2 for $[NO_2]_o$ = 25 ppm and $[O_3]_o$ = 10 ppm.

3.4.2 Experimental Procedures

The attendant measurements required to follow the reaction include: (1) initial concentrations and flow rates, (2) the $[O_3]$ as the sample leaves the reaction vessel so that the extent of the reaction (c.f., Figure 3-2) can be determined, and (3) the $[NO_2]$ as the sample leaves the reaction vessel so that the stoichiometry can be determined. The latter measurement must be made by a technique that does not destroy either NO_3 or N_2O_5 (e.g., IR absorption). The transit time of the sample between the reaction vessel and the appropriate monitor must be known or be small compared to the residence time of the sample in the reaction vessel.

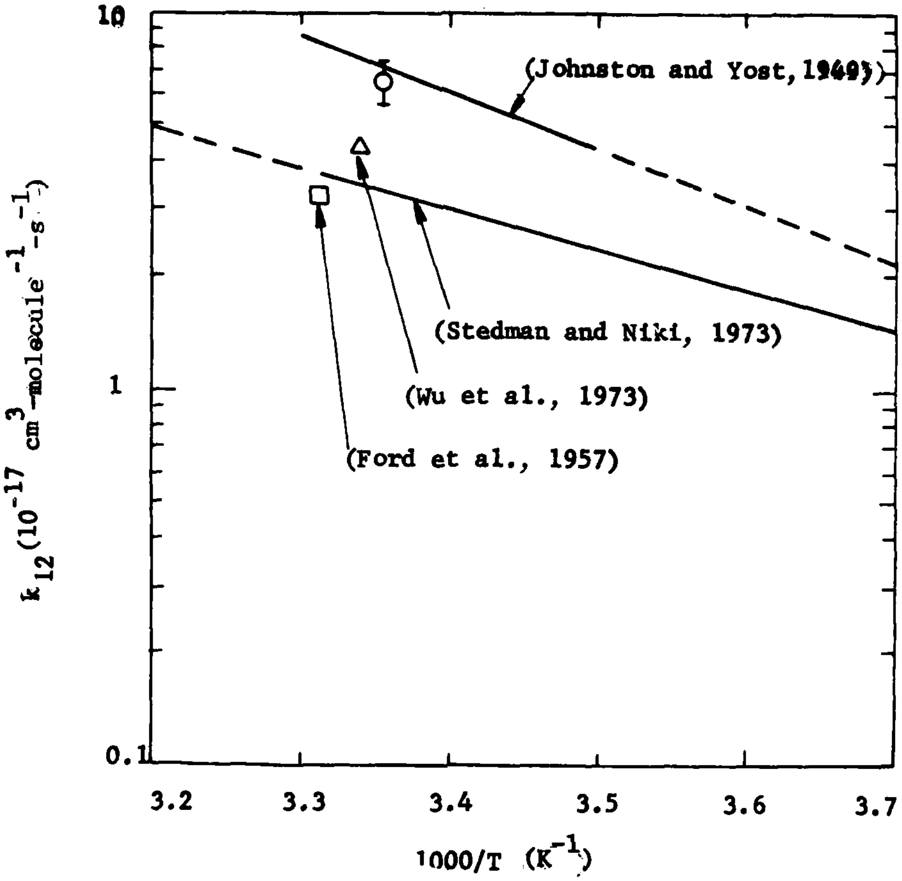


Figure 3-1. Arrhenius Plot For NO_2-O_3 Reaction

Kinetic runs were carried out initially at 0.25 and 0.50 SLPM with 13.1 ppm NO_2 and 26.0 and 13.0 ppm O_3, respectively, prior to dilution by the carrier of the other reactant. Subsequent tests were made at a total flow rate of 2.1 SLPM yielding a residence time of about 408 seconds. The reaction vessel volume of 14.3 liters and surface-to-volume ratio of 0.4 cm^{-1} consisted of a 1 liter stainless steel sampling cylinder with concentric counter flow tubing, a 7.8 liter stainless steel vessel and a 5.5 liter PTFE-lined vessel with AgCl windows that also served as a 20 meter White cell for IR absorption measurements. Measurements were usually carried out with a pathlength of 15.75 meters. The stainless steel vessels were vacuum baked prior to ozone conditioning of the walls and flow of the reactants. The above conditioning usually lasted for several hours. Flow rates were controlled by Tylan FC-260 flow controllers. These units were modified slightly by substituting

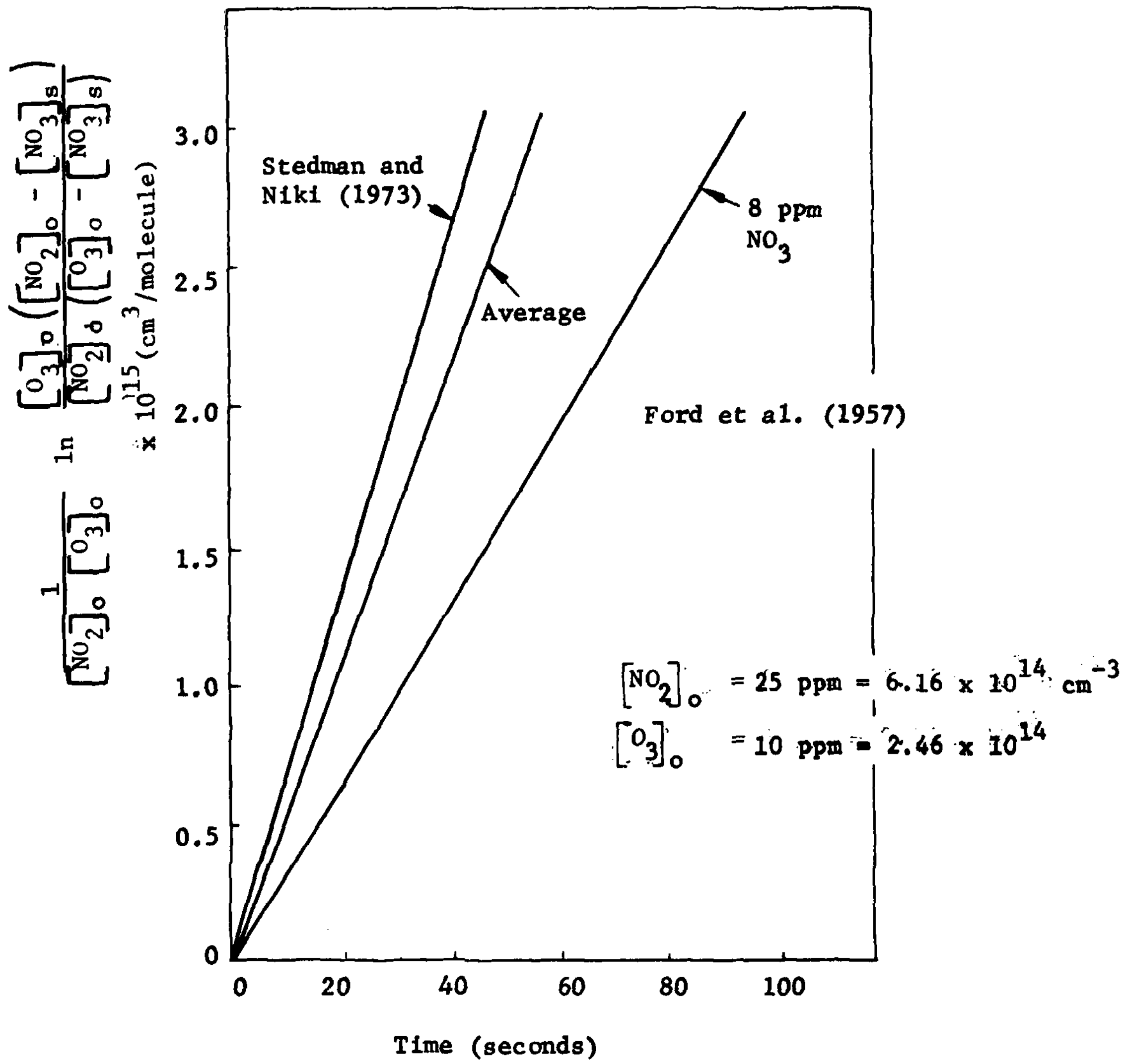


Figure 3-2. NO_3 Generation versus Time (T = 298 K)

PTFE O-rings for Viton O-rings. Steady-state flow conditions were usually reached after about 20 minutes. Infrared transmittances over the 1800-1000 cm^{-1} spectral range of the White cell contents were employed to follow the course of the reaction. As the flowing system desiccated itself with use, the relative amount of HNO_3 decreased substantially and improved the N_2O_5 yield and standard deviation.

The initial quantitative tests are tabulated in Table 3-9. The measured stoichiometry of 1.86 ±0.06 is in excellent agreement with the work of Wu

TABLE 3-9. N_2O_5 GENERATION AND STOICHIOMETRY MEASUREMENTS [(a)]

Expt. No.	$[O_3]_i$	$[O_3]_f$	$[NO_2]_i$	$[NO_2]_f$	$\Delta NO_2/\Delta O_3$	$[N_2O_5]$	Yield %	$[HNO_3]$	Rate Constant (ppm^{-1}-s^{1})
4	2.66	0.087	15.1	10.0	1.90	0.60	23		
5[(b)]	0.0	0.0	15.9	14.2	?	0.37	41		
8	6.45	2.15	12.0	3.70	1.93	2.79	65	0.30	1.276, 1.323×10^{-3}
9	7.20	2.40	12.0	2.90	1.90	2.39	50		1.60, 1.69
10	7.10	2.15	12.9[(c)]	3.94	1.82	2.67	54		1.30, 1.43
6	9.50	6.30	5.63	0.0	1.76	1.42	44		
7	9.40	5.45	7.39	0.0	1.87	1.96	50		
Mean ± SD					1.86±0.06				$(1.44 \pm 0.17) \times 10^{-3}$

(a) Concentrations in ppm units (= 2.4×10^{13} molecules/cm^3).

(b) For this test 10 ppm NO was also present as an initial reactant and consumed 9.4 ppm O_3 introduced as an initial reactant. This left 0.6 ppm NO by calculation vs a measured quantity of 0.62 ppm NO. The source of 0.37 ppm N_2O_5 is not clearly understood.

(c) The average for previous workers is $(1.32 \pm 0.43) \times 10^{-3}$ $ppm^{-1}s^{-1}$ at T = 298 K.

et al. (1973) and Graham (1975) shown in Figure 3-3. For a flow tube reactor operated with homogeneous mixing the rate constant for the reaction can be obtained from the steady-state concentrations of the reactions. For the rate limiting oxidation of NO_2 by O_3 the expression for the rate is given by:

$$k_{11} = \frac{-\frac{Q}{V}\left(-\Delta NO_2\right)}{2\left[NO_2\right]_f\left[O_3\right]_f} = \frac{-\frac{Q}{V}\left(-\Delta O_3\right)}{\left[NO_2\right]_f\left[O_3\right]_f} \qquad (3\text{-}17)$$

where the factor of 2 denotes the ideal stoichiometry, Q the flow rate, and f the final or steady-state concentration. Where determinant, the two rates are listed in Table 3-9 in the last columns. The value of (1.44 ±0.17) x 10^{-3} $ppm^{-1}s^{-1}$ is in excellent agreement with the work of others. The measured N_2O_5 yield compared to the theoretical yield based upon the stoichiometry and consumption of reactants has improved from about 23 percent to 65 percent. N_2O_5 is easily hydrolyzed by water forming nitric acid as a product. As it is usually a heterogeneous wall reaction, reconciliation of the odd-nitrogen budget is impossible. Circumvention of this problem to date has used in-situ IR absorption.

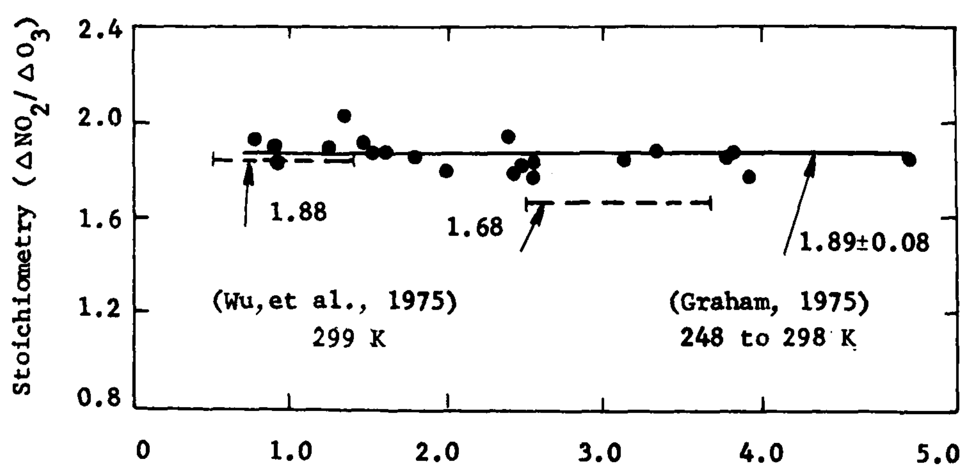


Figure 3-3. Plot of Measured Stoichiometries versus Initial Reactant Ratio For NO_2-O_3 Experiments

3.5 NITROUS PENTOXIDE (N_2O_5) THERMAL CONVERSION

3.5.1 Theory

The thermal conversion of N_2O_5 is a complex reaction with a net stoichiometric reaction:

$$2N_2O_5 \longrightarrow 4NO_2 + O_2 \qquad (16)$$

When NO, NO_2, and O_3 are present N_2O_5 can either be converted, generated, or serve as a catalyst according to the following net stoichiometric reactions:

$$NO + N_2O_5 \longrightarrow 3NO_2 \qquad (14)$$

$$2NO_2 + O_3 \longrightarrow N_2O_5 + O_2 \qquad (17)$$

$$2O_3 + N_2O_5 \longrightarrow 3O_2 + N_2O_5 \qquad (18)$$

Reaction 16 will be treated first. The governing mechanistic reactions for reaction 16 are the decomposition and recombination of N_2O_5 followed by two simultaneous bimolecular reaction paths, one of which has a fast sequential reaction converting NO, if present. These reactions are (H.S. Johnston, 1951):

$$N_2O_5 \xrightarrow{[(M)]} NO_2 + NO_3 \qquad (-13)$$

$$NO_2 + NO_3 \xrightarrow{[(M)]} N_2O_5 \qquad (13)$$

$$NO_2 + NO_3 \longrightarrow NO + NO_2 + O_2 \qquad (19)$$

$$NO + NO_3 \longrightarrow 2NO_2 \qquad (\ 7)$$

$$NO_3 + NO_3 \longrightarrow 2NO_2 + O_2 \qquad (20)$$

Rate limiting is governed by reactions (19) and (20).

The pyrolytic kinetics of these reactions have been studied by Schott and Davidson (1958) for temperatures greater than 450 K with argon as a diluent. The dissociation reaction of N_2O_5 is unimolecular, close to its second-order low pressure limit. The differential rate equation is given by:

$$\frac{d\,[N_2O_5]}{dt} = k_{-13}\,[M]\,[N_2O_5] \qquad (3\text{-}18)$$

with $k_{-13} = 5.0 \times 10^{13} \exp(-16,500 + 700/RT)\ (mol/l)^{-1}\text{-}s^{-1}$. At a pressure of 1 atmosphere and a temperature of 600 K, the concentration of the diluent $[M]$ is 2.01×10^{-2} mol/l and $k_{-13} = 4.85 \times 10^{7} (mol/l)^{-1}\text{-}s^{-1}$. At a reduced temperature of 400 K, $k_{-13} = 4.77 \times 10^{4}\ (mol/l)^{-1}\text{-}s^{-1}$. Integration of the above expression leads to:

$$[NO_2] = [N_2O_5] \left\{1 - \exp \left(-k_{-13}[M]\right) t\right\} \tag{3-19}$$

or a half-life of

$$\text{Half-Life} = \frac{\ln 2}{k_{-13}[M]} = 0.70 \text{ s for 600 K and} \tag{3-20}$$

$$= 0.48 \text{ ms for 400 K}$$

For the conditions of the stratosphere, the half-life is given below in Table 3-10.

TABLE 3-10. PREDICTED HALF-LIFE OF N_2O_5 IN A 400 K THERMAL CONVERTER

H (km)	P (atm)	$[M]$ (mol/l)	$\frac{\ln 2}{k_{-13}[M]}$ (s)
10	0.262	8.0×10^{-3}	1.8×10^{-3}
15	0.119	3.6	4.0
20	0.054	1.6	9.0
25	0.025	7.6×10^{-4}	1.9×10^{-2}
30	0.012	3.7	3.9
35	0.0057	1.7	8.5
40	0.0027	8.2×10^{-5}	1.8×10^{-1}

If the O_2 and N_2 molecules of the stratosphere take on the same role as the argon, then nearly complete conversion of N_2O_5 will occur if the residence time in the converter is about one second. A constant volume pump with a flow rate of 2.0-2.5 l/s requires a volume of 2.0 to 2.5 liters.

As cleanliness of the cell is a requirement to render heterogeneous wall reactions to negligible level, the converter volume-to-surface (V/S) ratio becomes important. Assuming a 2.5 cm diameter converter, the length required would be about 2 meters to obtain the necessary volume. If, however, the converter is designed to the 35 km specification limit; the residence time is set to four half-lives (94 percent conversion); and the diameter is increased to 5 cm, then the length becomes 35 cm for a 2 liter/s flow rate. The respective V/S ratios for the above converters are 0.61 and 1.23 cm, respectively.

Returning to the simultaneous bimolecular reactions with $k_7 \gg k_{19}$, the differential rate equation for the intermediary, NO_3 is given by

$$-\frac{d\left[NO_3\right]}{dt} = 2k_{19}\left[NO_2\right]\left[NO_3\right] + 2\,k_{20}\left[NO_3\right]^2 \qquad (3\text{-}21)$$

For a given reaction chamber, assuming steady-state conditions, a rate relation is written as:

$$R_{NO_3} = \frac{Q}{V}\left(\left[NO_3\right]_i - \left[NO_3\right]_s\right) \qquad (3\text{-}22)$$

where R_{NO_3} is the rate of disappearance of NO_3, Q is the flow rate, V is the reaction volume, and the subscripts i and s denote initial and steady-state conditions. The ratio Q/V has the units of s^{-1} and is inversely related to residence time.

Combining the two rate equations and dividing by $2\left[NO_2\right]\left[NO_3\right]$ yields,

$$k_{19} + k_{20}\frac{\left[NO_3\right]}{\left[NO_2\right]} = \frac{1}{t}\,\frac{\left[NO_3\right]_i - \left[NO_3\right]_s}{2\left[NO_2\right]\left[NO_3\right]} \qquad (3\text{-}23)$$

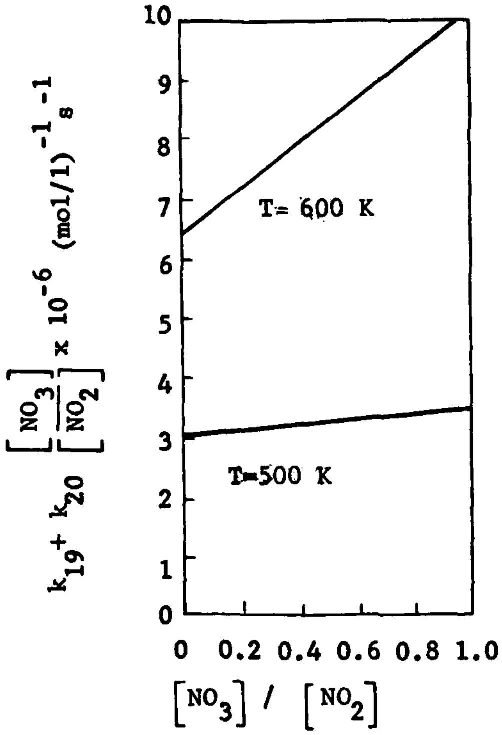
where

$$\log k_{19} = -\,(965 \pm 150)/T + 8.41 \qquad (3\text{-}24)$$

and

$$\log\ k_{19} + k_{20} = -\,(1403 \pm 60)/T + 9.34 \qquad (3\text{-}25)$$

The left-hand side of the rate equation is shown graphically in Figure 3-4 as a function of $\left[NO_3\right]/\left[NO_2\right]$ for T = 500 K and 600 K. The intercept at



T	k_{19}	$k_{19} + k_{20}$
500	3.02×10^6	3.42×10^6
600	6.33×10^6	10.04×10^6

Figure 3-4. Simultaneous Rate Constants at T = 500 and 600 K

a concentration ratio of zero corresponds to k_{19} and the intercept at unity ratio corresponds to $k_{19} + k_{20}$ or the apparent bimolecular rate constant at the beginning of the reaction. The slope of the function is k_{20}.

The rate equation can be rearranged to plot the concentration ratio versus time for given temperature and initial concentration conditions. This ratio is shown in Figure 3-5 for initial conditions of 10 ppm and a total pressure of 1 atmosphere.

For conditions more appropriate to the stratosphere, the terms of the rate equation are presented in Table 3-11 for initial conditions of 20 ppb N_2O_5, an ambient pressure of 0.1 atm and a 400 K thermal converter.

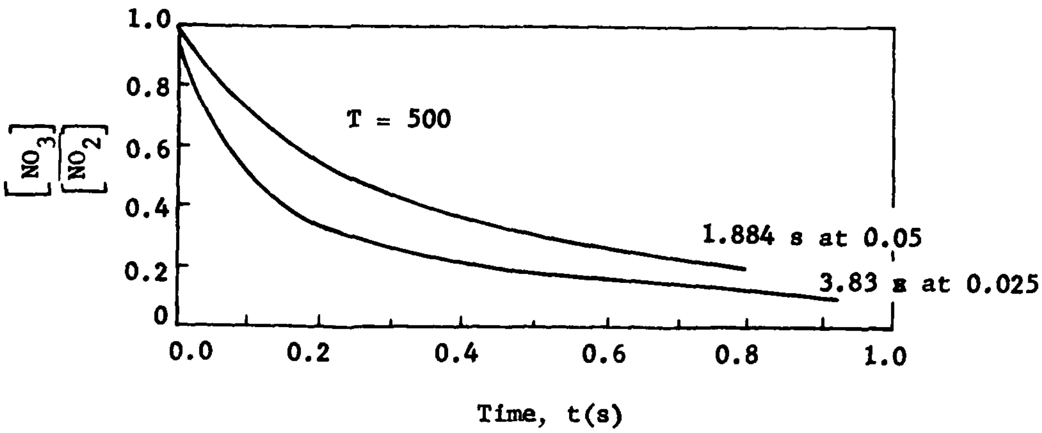


Figure 3-5. $[NO_3]$ Decay versus Time

TABLE 3-11. NO_3 RATE LIMITING DECAY

$[NO_3]$ (ppb)	$[NO_2]$ (ppb)	$\Delta[NO_3]$ (ppb)	$\frac{[NO_3]}{[NO_2]}$	t (s)
10.0	10.0	0	1.0	0
9.473	10.526	0.526	0.9	8.27×10^2
8.889	1.111	1.111	0.8	1.78×10^3
8.235	11.765	1.765	0.7	2.94×10^3
7.500	12.500	2.500	0.6	4.38×10^3
6.667	13.333	3.333	0.5	6.25×10^3

For Figure 3-5 or Table 3-11 it can be clearly seen that the ratio $[NO_3] / [NO_2]$ will be approximately unity for residence times of a few seconds or less and concentrations of a few ppb or less. The thermally converted N_2O_5 sample must then be analyzed as NO_2 or NO_3, or a second conversion of either constituent must occur followed by detection of the end products. The stoichiometry of these conversions, however, must be known.

For reaction 16 the growth of NO_2 is given by:

$$\frac{d\left[NO_2\right]}{dt} = k_{-13}\left[N_2O_5\right] - k_{13}\left[NO_2\right]\left[NO_3\right] + 2k_{13}\left[NO\right]\left[NO_3\right] \tag{3-26}$$

and the growth of the NO_3 radical is

$$\frac{d\left[NO_3\right]}{dt} = k_{-13}\left[N_2O_5\right] - \left(k_{13} + k_{19}\right)\left[NO_2\right]\left[NO_3\right] - k_{13}\left[NO\right]\left[NO_3\right] \tag{3-27}$$

Since NO will generally be present, the net stoichiometric reaction must also be considered:

$$NO + N_2O_5 \longrightarrow 3NO_2 \tag{13}$$

For this reaction and for lower temperatures, a steady-state approximation for the $\left[NO_3\right]$ intermediary is made, i.e., $\frac{d\left[NO_3\right]}{dt} = 0$. With this approximation the growth of NO_2 is given by:

$$\frac{d\left[NO_2\right]}{dt} = k_{-13}\left[N_2O_5\right]\frac{k_{19}\left[NO_2\right] + 3k_7\left[NO\right]}{\left(k_{13} + k_{19}\right)\left[NO_2\right] + k_7\left[NO\right]} \tag{3-28}$$

with the knowledge that $k_7 >> k_{19}$ (pg. 38), this expression can be simplified to;

$$\frac{d\left[NO_2\right]}{dt} = 3\,k_{-13}\left[N_2O_5\right]\frac{\left[NO\right]}{\left[NO\right] + k_{13}/k_7\left[NO_2\right]} \tag{3-29}$$

Since $\left[NO\right] \approx \left[NO_2\right]$ in the stratosphere and k_{13} at 400 K is $<< k_7$, $k_7\left[NO\right]$ will be much greater than $k_{13}\left[NO_2\right]$. For these conditions, a first-order rate for reaction 14 will simply be that of the elementary unimolecular rate given for reaction -13.

The third reaction listed in this section is restated;

$$2NO_2 + O_3 \longrightarrow N_2O_5 + O_2 \tag{17}$$

and has been observed (Section 3.4.1) to be second-order in reactants. The mechanism is simply

$$2NO_2 + O_3 \longrightarrow NO_3 + O_2 \tag{12}$$

$$NO_2 + NO_3 \longrightarrow N_2O_5 \tag{13}$$

Applying the steady-state assumption for NO_3, the loss rate for O_3 is simply

$$-\frac{d\left[O_3\right]}{dt} = k_1\left[NO_2\right]\left[NO_3\right] \; . \tag{3-30}$$

The fourth reaction listed in this section is restated:

$$2O_3 + N_2O_5 \longrightarrow 3O_2 + N_2O_5 \tag{18}$$

This reaction is the well-known N_2O_5 catalytic decomposition of O_3. The governing mechanistic reactions for reaction (18) are:

$$NO_2 + O_3 \longrightarrow NO_3 + O_2 \tag{12}$$

$$NO_2 + NO_3 \xrightarrow{(M)} N_2O_5 \tag{13}$$

$$2NO_3 \longrightarrow 2NO_2 + O_2 \tag{20}$$

$$N_2O_5 \longrightarrow NO_2 + NO_3 \tag{-13}$$

If the pseudo-reference species, NO_2 and NO_3, are equilibrated with N_2O_5, they are treated kinetically as though they were intermediaries in a consecutive process. This leads to the following differential rate equation:

$$-\frac{d\left[O_3\right]}{dt} = 2\left(\frac{k_{-13}^{2}\, k_{11}^{2}\, k_{19}}{4k_{13}}\right)^{1/3} \left[N_2O_5\right]^{2/3} \left[O_3\right]^{2/3} \tag{3-31}$$

3.5.2 Stratospheric-Based Instrument Modeling

The above reactions plus the ozone oxidation of NO to NO_2 and NO_2 to NO_3 have been modeled using the EPISODE adaptation of the GEARS code (Gear, 1971 and Hindmarsh, 1975). These codes are chemical kinetics programs that solve coupled stiff differential equations. The solutions are obtained by implicit linear multisteps. With the GEAR code, fixed-step formulae are employed with changes in step, when required, by interpolation. In contrast, the EPISODE code is based upon formulae that are of variable step size. This feature

lends stability to the solution. Given the correct set of chemical reactions, the solutions tend to be an exact representation of the products and reactants for homogeneous reactions.

Table 3-12 provides printouts for a 400 K converter with input concentrations set for H = 15 km and H = 25 km. The initial concentrations can be read from the respective first lines at t = 0. Within the first half-second most of the N_2O_5 is converted to NO_2 and NO_3. Subsequently $[NO_2]$ increases to a steady-state level of 9.6×10^9 molecules/cm^3 and 7.2×10^9 molecules/cm^3; $[NO_3]$ increases at a slower rate to a steady-state level of 3.5×10^8 molecules/cm^3 and 1.1×10^9 molecules/cm^3; and $[NO]$ decays. As an example of the $[NO_x]$ budgeting, refer to the case for H = 25 km and t = 5.0 s. These values are given in Table 3-13.

Although the data of Table 3-13 shows acceptable accounting or budgeting of $\Delta[NO_x] = \Delta[NO_2] + \Delta[NO]$ from redox reactions the data does not permit an accurate measurement of $[N_2O_5]$. The principal reason is that some of the unmeasured $[NO_3]$ is converted to NO_2 via reaction -13. This in effect alters specificity. If the measurement could be carried out in 2 seconds, the $\Delta[NO_3]$ error would be reduced by about 33 percent for the case cited.

From the example cited in Table 3-13, setting aside for the moment the above mentioned problem, a quantitative measure of $[N_2O_5]$ may be obtained, if the following conditions are met: (1) N_2O_5 is not lost to the instrumentation walls, (2) $NO_x = NO + NO_2$ was determined accurately, (3) the $[NO_3]$ from both the ambient stream and as an N_2O_5 decomposition product is quantitatively converted to NO_x prior to being measured as NO, and (4) the NO-NO_2 instrumentation did not convert any of the ambient N_2O_5 during sample residence. This latter statement is a specificity condition. The third condition is treated next.

Of the intermediary, NO_3 entering an NO_2 photolytic cell, some may be converted according to the spectral energy available as given by Johnston and Graham (1974):

TABLE 3-12. HAPP RESIDENCE TIME STUDY

T = 400 K

HAPP RESIDENCE TIME STUDY **H = 15 km**

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	1.000D 07	5.000D 09	2.000D 06	5.000D 09	3.000D 12	8.100D 17	1.300D 09	1.000D 06	6.000D 12
0.50	1.196D 02	5.412D 09	1.349D 07	4.597D 09	3.000D 12	8.100D 17	1.300D 09	8.390D 05	6.000D 12
1.00	1.418D 02	5.781D 09	1.509D 07	4.226D 09	2.999D 12	8.100D 17	1.300D 09	7.046D 05	6.000D 12
1.50	1.674D 02	6.120D 09	1.682D 07	3.886D 09	2.999D 12	8.100D 17	1.300D 09	5.941D 05	6.000D 12
2.00	1.952D 02	6.431D 09	1.867D 07	3.572D 09	2.999D 12	8.100D 17	1.300D 09	5.033D 05	6.000D 12
2.50	2.253D 02	6.717D 09	2.061D 07	3.284D 09	2.998D 12	8.100D 17	1.300D 09	4.286D 05	6.000D 12
3.00	2.574D 02	6.980D 09	2.266D 07	3.019D 09	2.998D 12	8.100D 17	1.300D 09	3.670D 05	6.000D 12
3.50	2.915D 02	7.221D 09	2.480D 07	2.776D 09	2.998D 12	8.100D 17	1.300D 09	3.163D 05	6.000D 12
4.00	3.275D 02	7.443D 09	2.703D 07	2.552D 09	2.998D 12	8.100D 17	1.300D 09	2.745D 05	6.000D 12
4.50	3.654D 02	7.647D 09	2.935D 07	2.346D 09	2.997D 12	8.100D 17	1.300D 09	2.400D 05	6.000D 12
5.00	4.049D 02	7.834D 09	3.174D 07	2.157D 09	2.997D 12	8.100D 17	1.300D 09	2.115D 05	6.000D 12
5.50	4.460D 02	8.005D 09	3.420D 07	1.982D 09	2.997D 12	8.100D 17	1.300D 09	1.879D 05	6.000D 12
6.00	4.886D 02	8.163D 09	3.674D 07	1.822D 09	2.997D 12	8.100D 17	1.300D 09	1.684D 05	6.000D 12
6.50	5.326D 02	8.307D 09	3.935D 07	1.675D 09	2.997D 12	8.100D 17	1.300D 09	1.522D 05	6.000D 12
7.00	5.780D 02	8.440D 09	4.202D 07	1.540D 09	2.997D 12	8.100D 17	1.300D 09	1.387D 05	6.000D 12
7.50	6.245D 02	8.562D 09	4.475D 07	1.415D 09	2.996D 12	8.100D 17	1.300D 09	1.276D 05	6.000D 12
8.00	6.722D 02	8.673D 09	4.754D 07	1.301D 09	2.996D 12	8.100D 17	1.300D 09	1.183D 05	6.000D 12
8.50	7.209D 02	8.776D 09	5.039D 07	1.196D 09	2.996D 12	8.100D 17	1.300D 09	1.105D 05	6.000D 12
9.00	7.706D 02	8.869D 09	5.329D 07	1.099D 09	2.996D 12	8.100D 17	1.300D 09	1.040D 05	6.000D 12
9.50	8.213D 02	8.955D 09	5.624D 07	1.010D 09	2.996D 12	8.100D 17	1.300D 09	9.854D 04	6.000D 12
10.00	8.728D 02	9.034D 09	5.924D 07	9.286D 08	2.996D 12	8.100D 17	1.300D 09	9.396D 04	6.000D 12

HAPP RESIDENCE TIME STUDY **H = 25 km**

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	7.000D 08	6.200D 09	2.000D 06	7.000D 08	4.300D 12	1.700D 17	3.000D 09	1.000D 06	6.000D 12
0.50	9.128D 05	6.982D 09	7.012D 08	6.173D 08	4.300D 12	1.700D 17	3.000D 09	8.384D 05	6.000D 12
1.00	9.252D 03	7.056D 09	7.022D 08	5.438D 08	4.300D 12	1.700D 17	3.000D 09	6.556D 05	6.000D 12
1.50	8.164D 03	7.120D 09	7.027D 08	4.791D 08	4.300D 12	1.700D 17	3.000D 09	5.165D 05	6.000D 12
2.00	8.239D 03	7.176D 09	7.037D 08	4.221D 08	4.300D 12	1.700D 17	3.000D 09	4.106D 05	6.000D 12
2.50	8.312D 03	7.225D 09	7.050D 08	3.719D 08	4.300D 12	1.700D 17	3.000D 09	3.300D 05	6.000D 12
3.00	8.381D 03	7.267D 09	7.067D 08	3.277D 08	4.300D 12	1.700D 17	3.000D 09	2.686D 05	6.000D 12
3.50	8.448D 03	7.304D 09	7.087D 08	2.888D 08	4.300D 12	1.700D 17	3.000D 09	2.219D 05	6.000D 12
4.00	8.513D 03	7.336D 09	7.110D 08	2.545D 08	4.300D 12	1.700D 17	3.000D 09	1.862D 05	6.000D 12
4.50	8.575D 03	7.364D 09	7.135D 08	2.243D 08	4.299D 12	1.700D 17	3.000D 09	1.591D 05	6.000D 12
5.00	8.636D 03	7.388D 09	7.162D 08	1.977D 08	4.299D 12	1.700D 17	3.000D 09	1.384D 05	6.000D 12
5.50	8.694D 03	7.409D 09	7.190D 08	1.743D 08	4.299D 12	1.700D 17	3.000D 09	1.226D 05	6.000D 12
6.00	8.752D 03	7.426D 09	7.220D 08	1.536D 08	4.299D 12	1.700D 17	3.000D 09	1.106D 05	6.000D 12
6.50	8.808D 03	7.441D 09	7.252D 08	1.354D 08	4.299D 12	1.700D 17	3.000D 09	1.014D 05	6.000D 12
7.00	8.863D 03	7.454D 09	7.284D 08	1.194D 08	4.299D 12	1.700D 17	3.000D 09	9.441D 04	6.000D 12
7.50	8.917D 03	7.465D 09	7.318D 08	1.053D 08	4.299D 12	1.700D 17	3.000D 09	8.905D 04	6.000D 12
8.00	8.971D 03	7.474D 09	7.353D 08	9.290D 07	4.299D 12	1.700D 17	3.000D 09	8.496D 04	6.000D 12
8.50	9.023D 03	7.481D 09	7.389D 08	8.197D 07	4.299D 12	1.700D 17	3.000D 09	8.183D 04	6.000D 12
9.00	9.075D 03	7.487D 09	7.425D 08	7.233D 07	4.299D 12	1.700D 17	3.000D 09	7.944D 04	6.000D 12
9.50	9.126D 03	7.492D 09	7.462D 08	6.385D 07	4.299D 12	1.700D 17	3.000D 09	7.761D 04	6.000D 12
10.00	9.176D 03	7.496D 09	7.499D 08	5.638D 07	4.299D 12	1.700D 17	3.000D 09	7.620D 04	6.000D 12

TABLE 3-13. NO_x BUDGET

(for Table 3-12, H = 25 km, T = 400 K, t = 5.0 s)

Species	Decomposition	Species	Combination
ΔN_2O_5	-7.000×10^8	ΔNO_x	$+ 6.86 \times 10^8$
ΔNO_2	7.000×10^8		
ΔNO_3	7.142×10^8		
$\Delta N_2O_5 - \Delta NO_3$	-0.142×10^8		
Total ΔNO_x	6.858×10^8	Total NO_x	$+ 6.86 \times 10^8$

$$NO_3 + h\nu \longrightarrow NO_2 + O(^3P) \quad \lambda < 578 \text{ nm} \qquad (21)$$

$$NO_3 + h\nu \longrightarrow NO + O_2(^1\Sigma) \quad \lambda > 578 \text{ nm} \qquad (22)$$

There is conjecture, however, that $NO + O_2(^1\Sigma)$ products also may be formed for wavelengths less than 578 nm.

Photoabsorption cross-sections to $\lambda \geq 470$ nm and quantum yields in the visible have been determined for reactions 21 and 22 (Graham, 1975). The quantum yields, wavelength averaged cross-sections, and light distributions are given below in Table 3-14. From the fourth column of data it is apparent that the conjecture of the previous paragraph is valid. For a solar spectral distribution and zero zenith angle, Graham's computed rates are $J_{21} = 0.099 \pm 0.02 \text{ s}^{-1}$ and $J_{22} = 0.040 \pm 0.02 \text{ s}^{-1}$.

The products of reaction 22 will rapidly react as follows:

$$O(^3P) + NO_2 \longrightarrow NO + O_2 \qquad (6)$$

where

$$k_6 = 3.5 \times 10^{-12} \text{ cm}^3\text{-molecule}^{-1}\text{s}^{-1} \text{ (Kaufman, 1961)}$$

Since the NO_2 photolytic converter of paragraph 3.2 does not have any substantial flux at $\lambda > 470$ nm reaction 21 is not anticipated. NO_3 absorption cross-sections for $\lambda < 400$ nm, however, have not been measured.

TABLE 3-14. NO_3 FREE RADICAL PHOTOLYTIC TERMS

Parameter	Reaction				
	J_{21}	J_{21}	J_{21}	J_{22}	J_{22}
Quantum Yield	0.14	0.23	0.049	0.85	0.63
Avg σ NO_3: $\lambda \leq 580$ nm (cm^2/molec)	1.88×10^{-18}	2.51×10^{-18}		1.88×10^{-18}	2.51×10^{-18}
Avg σ NO_3 $\lambda > 580$	2.99	3.11	2.17×10^{-18}	2.99	3.11
Percent light, $\lambda \leq 580$ nm	93	37	0	93	37
Percent light, $\lambda > 580$	7	63	100	7	63
Integrated light intensity ($10^{16} h\nu/cm^2$-s)	1.55	1.07	0.33	1.55	1.07

Although an N_2O_5 measurement does not appear feasible due to specificity problems, some of which are deferred to paragraph 3.8, Potential Interferents, the thermal conversion of N_2O_5 was experimentally treated in the lab and is discussed in the next paragraph.

3.5.3 Experimental Procedures and Results

The thermal decomposition of nitrous pentoxide was studied using a stainless steel converter between the N_2O_5 generating apparatus and the long path absorption cell of the Model 580 spectrophotometer. The spectrophotometer enabled observation of the major constitutents involved in the thermal conversion process. A schematic of the apparatus is shown in Figure 3-6.

N_2O_5 was created by the gas phase reaction of NO_2 and O_3 in the presence of excess NO_2 in the same manner as described in paragraph 3.5.1. Several minor changes, however, were made to further reduce water contamination. Two test runs are discussed in detail.

The core of the converter consisted of a 2½-inch diameter x 2-inch long stainless steel block. The gas passed through a ½-inch diameter hole in the center of the block. A sintered stainless disk pressed into the gas channel permitted complete thermalization of the gas. The temperature of the block was monitored using platinum resistance sensors. A cartridge heater inserted into the block was the heat source. The block temperature was not regulated but stayed within ± 1 K during the course of each data run.

For the initial test run, pertinent conversion data of the reactants are presented in Table 3-15. The initial concentrations of $[NO_2]$ and $[O_3]$ prior to mixing were 23.5×10^{13} and 6.5×10^{13} molecules/cm^3, respectively. The final concentrations of $[NO_2]$ and $[O_3]$ were 11.3×10^{13} and zero molecules/cm^3. The ratio $\Delta[NO_2]/\Delta[O_3]$ is therefore 1.88, as expected. Although the IR scan of Figure 3-7 for T = 23 C shows little evidence of H_2O being present, the measured yield of N_2O_5 for this test, assuming a stoichiometry of 1.88, is only 43 percent. The remaining 57 percent appears as nitric acid which is evident at 1340 and 1315 cm^{-1}. The expected amount of HNO_3 based upon the 57 percent loss of N_2O_5 is 7.44×10^{13} molecules/cm^3. From Table 3-15, it can be seen about 71 percent of the HNO_3 appeared in the gas phase.

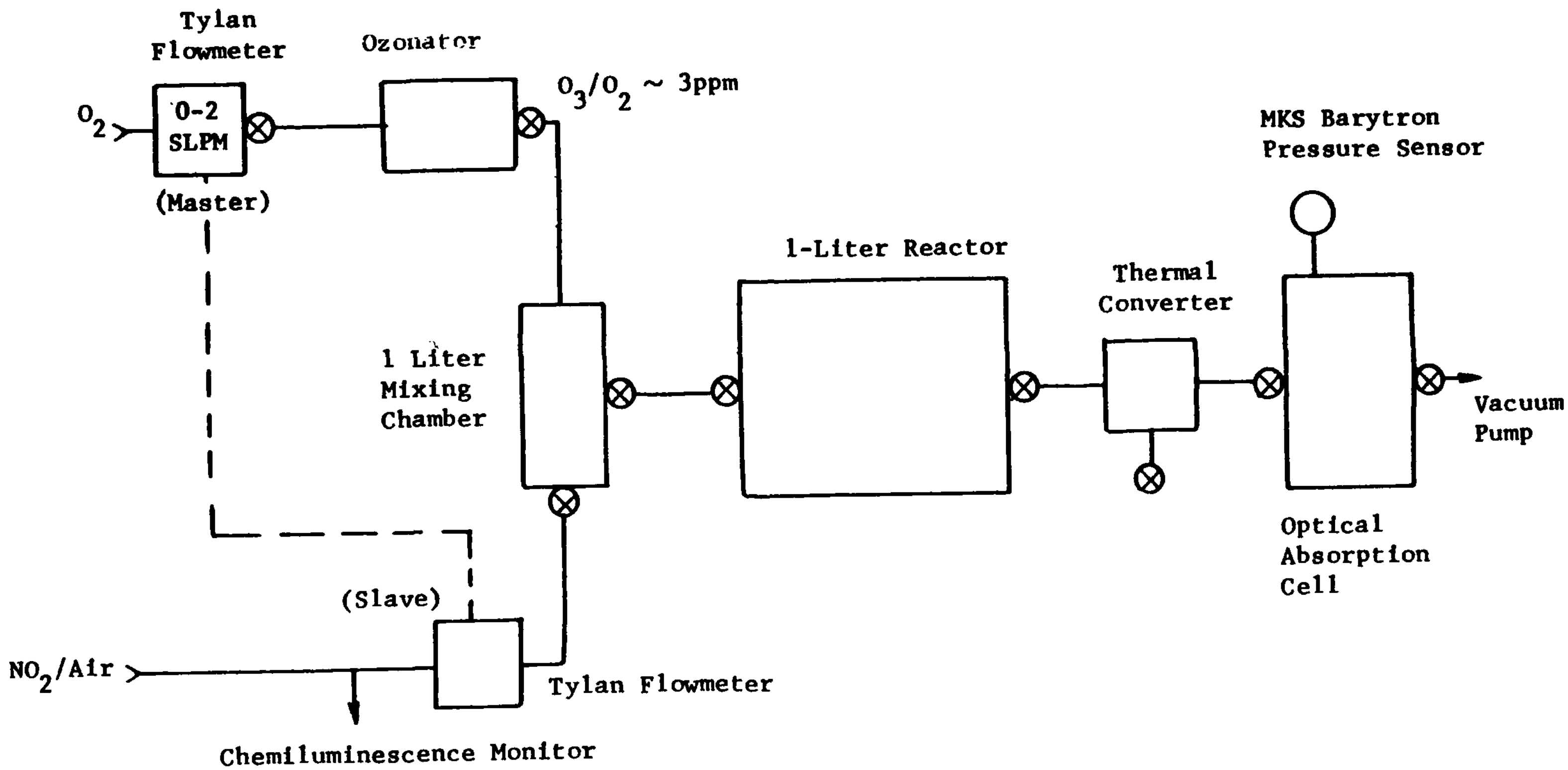
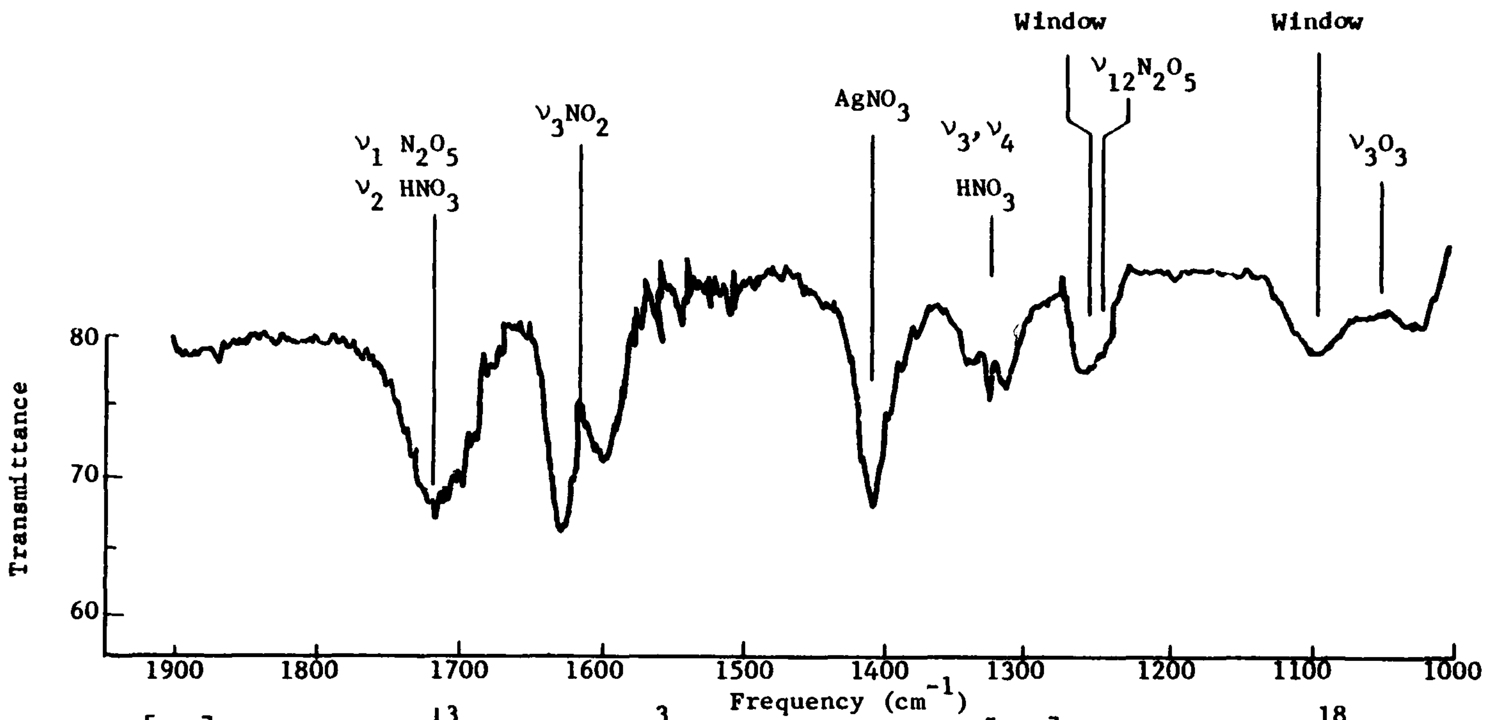


Figure 3-6. Setup for Experiment To Observe Thermal Decomposition of N_2O_5



$[NO_2]$ = 11.3×10^{13} molecules/cm^3

$[N_2O_5]$ = 2.8

$[HNO_3]$ = 5.3

$[O_3]$ $\simeq$ 0

$[NO_2]_i$ = 23.5×10^{18} molecules/cm^3

$[O_3]_i$ = 6.5

S = 1.89, Y = 43%

Resolution ~ 3.7 cm^{-1} Ordinate exp = 2T

Pathlength 15.75 m Q = 2 slpm T = 23°C
P = 760 torr

Figure 3-7. N_2O_5 Generation Spectra

TABLE 3-15. NO_2, N_2O_5 AND HNO_3 MEASURED CONCENTRATIONS VS THERMAL CONVERTER TEMPERATURE

Temp. (K)	NO_2	N_2O_5 x 10^{13} (molecules/cm^3)	HNO_3
298	11.3	2.78	5.32
373	13.1	1.63	7.67
473	18.8	0	5.62
523	17.8		5.96
573	21.7		3.87
623	21.9		1.84
673	25.3		0.71

For the initial testing of the N_2O_5 converter it was decided that a series of thermal tests at differing temperatures should be carried out. From the above table and a sample residence time of about 0.5 second, it can be seen that all of the N_2O_5 accounted for had decomposed at a temperature of 473 K. At this temperature, however, the data indicates that $\Delta[NO_2]$ is considerably greater than expected from a $\Delta[N_2O_5]$ of -2.78×10^{13} molecules/cm^3.

In addition, a review of the HNO_3 concentration versus temperature indicates that possibly HNO_3 is being desorbed from the converter walls at a temperature of 373 K. As the converter had been used on the two previous days, it is feasible that residual HNO_3 was present.

Finally, the high temperature NO_2 and HNO_3 data are of interest for the conversion of HNO_3 which is described in detail in paragraph 3.6. At a temperature of 673 K the NO_2 concentration was determined to be 25.3×10^{13} molecules/cm^3 as compared to the initial concentration of 23.5×10^{13} molecules/cm^3 prior to reaction with O_3 or about 1.8×10^{13} molecules/cm^3 too high. Undoubtedly this discrepancy contains experimental measurement errors but could also have arisen from the apparent desorbed HNO_3 which from the first two HNO_3 entries is seen to be about 2.3×10^{13} molecules/cm^3. Considering

the 523-673 K temperature range and making the $[NO_2] = 1.8 \times 10^{13}$ molecules/cm^3 correction, one has a $\Delta[NO_2]$ of 5.7×10^{13} molecules/cm^3 as compared to a $\Delta[HNO_3]$ of 5.25×10^{13} molecules/cm^3. Paragraph 3.6.1, to follow, discusses theoretically a stoichiometry of unity for the decomposition of HNO_3 to NO_2.

For the second test run emphasis was placed on repeatability and closer monitoring of thermal trends. The concentration of NO_2 prior to dilution was 58 ppm as determined by the chemiluminescence monitor. When diluted with the O_3/O_2 flow, the concentration of NO_2 was 15.7 ppm. The concentration determined by IR absorption was found to be 10 ppm. Ozone was generated by a standard UV lamp ozonator and grade 4.5 oxygen. The spectrum was analyzed using the data of Pitts (1976), c.f. Appendix A. The result was an ozone concentration of 3.3 ppm (NTP) or 3.2 ppm under laboratory conditions of 765 Torr and 26°C. The change in NO_2 concentration following reaction with the ozone was 8.0 ppm with all of the ozone being consumed. The ratio $[NO_2]/[O_3] = 2.5$ for these experiments.

The absorption spectrum of the reacted gases is shown in Figure 3-8. In addition to the NO_2 band at 1620 cm^{-1}, bands attributable to HNO_3 and N_2O_5 are clearly visible. The spectral run of Figure 3-8 extends the spectrum to lower frequencies to present the ν_{13} and ν_{14} bands of N_2O_5. Using the absorption crosssections given in Appendix A for HNO_3 at 1315 cm^{-1} and 1340 cm^{-1}, the concentration of HNO_3 was found to b 3.2×10^{13} molecules/cm^3 or 1.4 ppm. The maximum amount of N_2O_5 that could be generated would be equal to the amount of O_3 consumed which was 3.2 ppm. The nitric acid is believed to be formed by heterogeneous wall reactions of N_2O_5 with adsorbed water. The net reaction is

$$H_2O + N_2O_5 \longrightarrow 2HNO_3 \tag{23}$$

Thus, 1.4 ppm of HNO_3 represents the reaction of 0.7 ppm of N_2O_5. Using the absorption cross sections given in Appendix A for N_2O_5 at 1246 cm^{-1}, the concentration of N_2O_5 was found to be 4.6×10^{13} molecules/cm^3 or 2.0 ppm. This represents a yield of 59 percent with the loss of 0.7 ppm to heterogenously and homogeneously formed HNO_3. Thus the nominal N_2O_5 yield is 2.7/3.4 = 0.8 which is quite good.

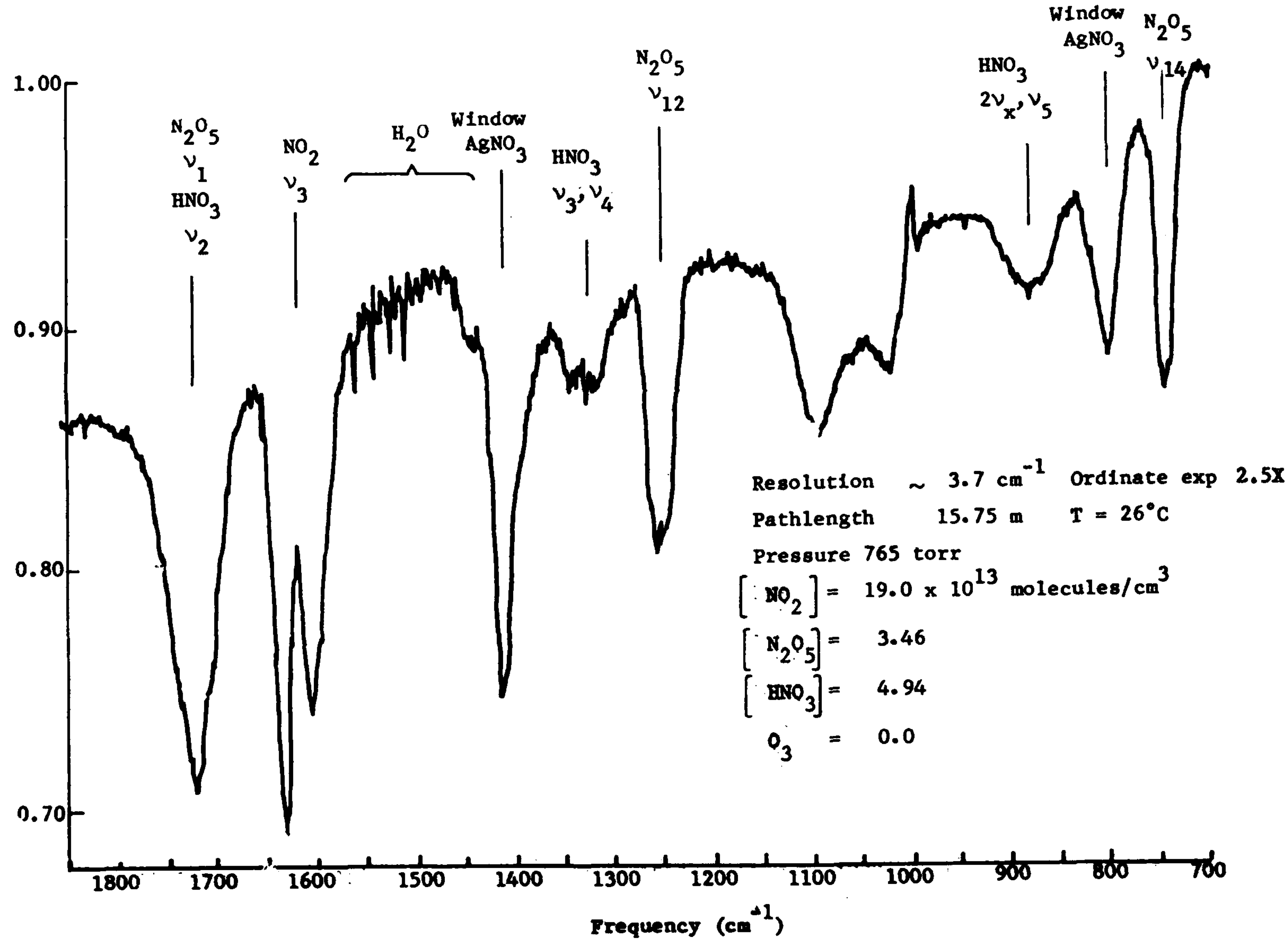


Figure 3-8. Absorption Spectra of N_2O_5 and HNO_3

The recorded data consisted of a least three complete spectral scans, similar to Figure 3-8, taken after the block had reached thermal equilibrium. The transmission at various distinct spectral features was recorded and compared to a reference spectrum (pure O_2). The absorbance was plotted as a function of temperature for these features of N_2O_5, HNO_3, and NO_2 (Figure 3-9). In addition, the N_2O_5-HNO_3 mixed feature at 1720 cm^{-1} was plotted (Figure 3-10). Examining these graphs, it is seen that the amount of N_2O_5 declines steadily with increasing temperatures. The nitric acid concentration peaks near 475 K, while the yield of NO_2 increases steadily to within 1 percent of its unreacted level. The "missing" NO_2 has probably been converted to NO although this was not explicitly checked. The standard deviation of the data was typically 0.1 to 0.3 percent indicating stable conditions during the successive spectral measurements.

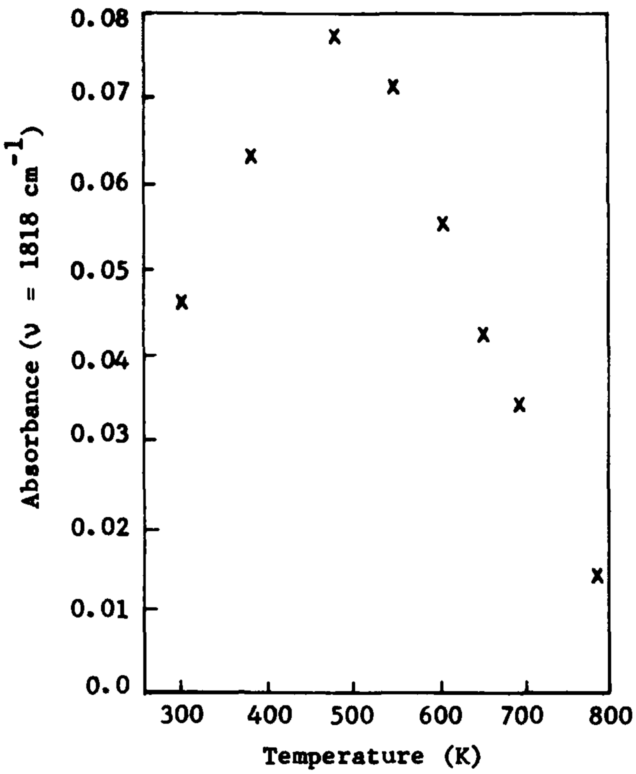
The complicated thermal behavior exhibited in these graphs is related to several factors. Primary among these is the time that the gas spends in the long path absorption cell ($\simeq$ 300 sec). This time is long enough to allow some reverse reactions to occur, especially in the oxygen-rich environment of these experiments. Also, the gas temperature in the absorption cell was not well determined. Nevertheless, almost total recovery of the NO_2 has been achieved, thus indicating > 99 percent conversion efficiency.

3.6 NITRIC ACID (HNO_3) GENERATION

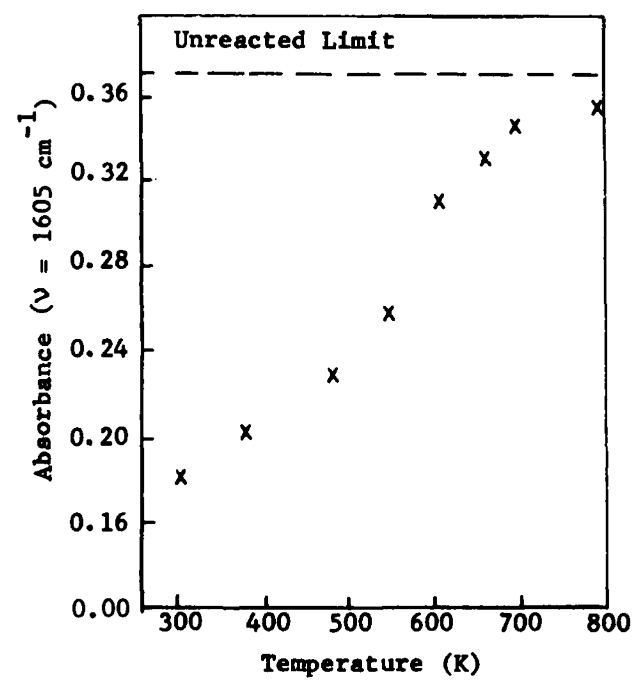
For nitric acid (HNO_3) synthesis, vapor diffusion of HNO_3 from an HNO_3/H_2SO_4/H_2O mixture was employed. This technique approximates the approach used by Stedman (1977).

3.6.1 Theory

Generation of HNO_3 is best carried out by the low pressure distillation of HNO_3/H_2SO_4 (Wilson and Miles, 1940) combined with a diffusion flow technique (Stedman, 1977). A ratio of 100 to 33.3 parts of concentrated 70% HNO_3/30% H_2O and H_2SO_4 was used to obtain weight percentages of HNO_3 = 49, H_2SO_4 = 30, and H_2O = 21. The vapor composition was greater than 98% HNO_3. A stream of dry nitrogen or dry air is then blown by the mouth of the flask to create ~ 3 ppm concentrations of HNO_3 in the flowing gas stream.

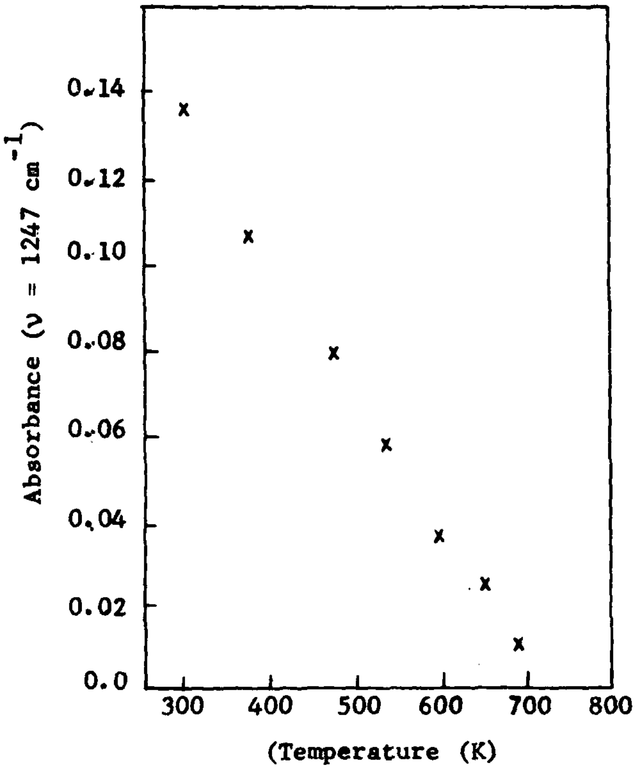


a. HNO_3 Absorbance

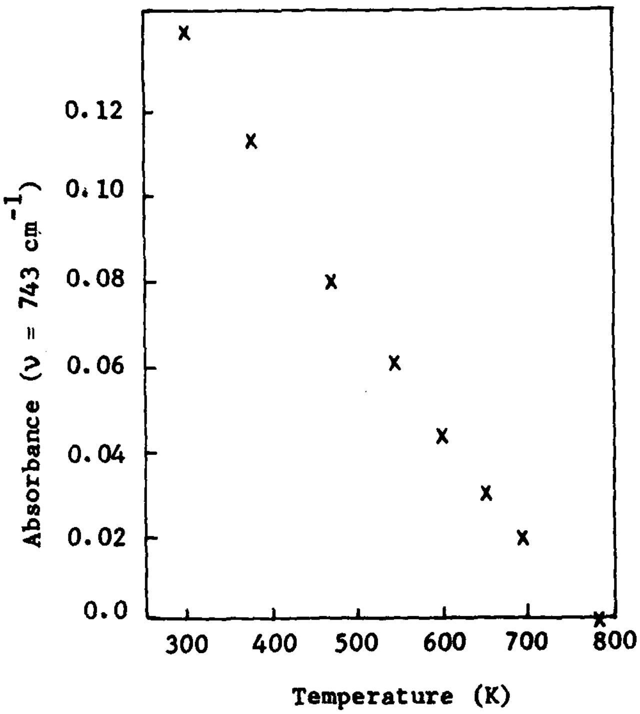


b. NO_2 Absorbance

Figure 3-9. Absorbances at Converter Output (1 of 2)



c. N_2O_5 Absorbance



d. N_2O_5 Absorbance

Figure 3-9. Absorbances at Converter Output (2 of 2)

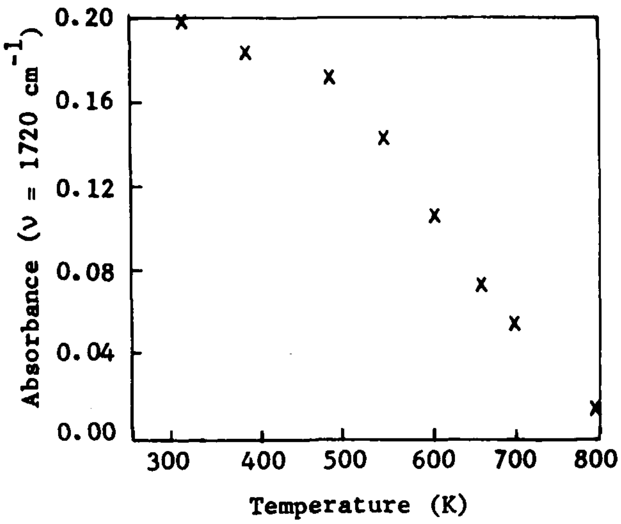


Figure 3-10. HNO_3 and N_2O_5 Absorbance at Converter Output

The vapor pressure of the HNO_3 was derived from boiling point data on Gibbs type ternary composition diagrams and plotted versus 1000/T shown in Figure 3-11. For diffusion flow samples of HNO_3, the solution was held at 35°C yielding a partial pressure of 34 torr. For high spectral resolution measurements at temperatures simulating those of the stratosphere, a differential pumping technique was employed and the Pascal-Saposchnikow data was extrapolated according to the integrated Clausius-Clapeyron expression:

$$\log P = \frac{0.05223A}{T} + B(\text{torr}),$$

where A = 45,568 and B = 9.259. This expression permits one to derive from total pressure measurements the saturated partial pressure of HNO_3 as a function of temperature.

Under diffusion flow, the predicted concentration at the upper end of the diffusion tube is given by the expression

$$C = \frac{10^6 \times q_d}{Q} \text{ (ppm)}.$$

where

$$q_d = \frac{DA}{L} \ln \frac{P}{P-P_{HNO_3}},$$

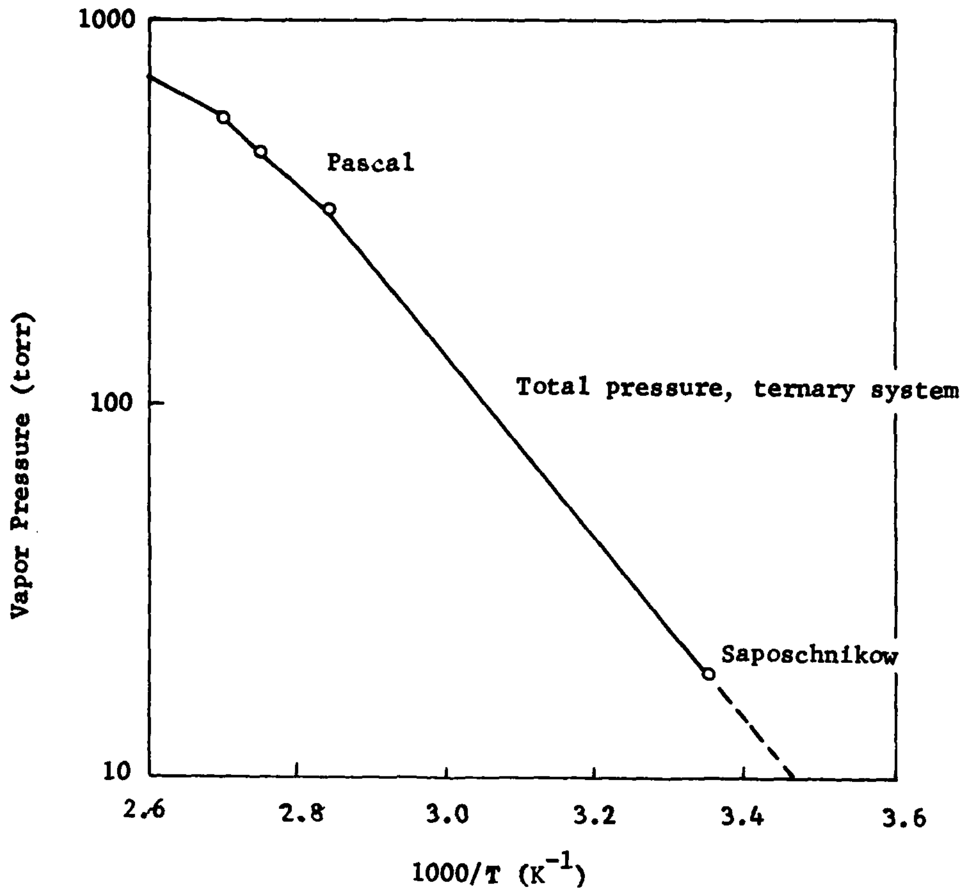


Figure 3-11. HNO_3 Vapor Pressure vs Reciprocal Temperature

and:

Q = flow rate (ml/s)

q_d = diffusion rate (ml/s)

D = diffusion coefficient $\approx 0.09 \left(\frac{306}{298}\right) \left(\frac{760}{747}\right)$ cm^2/sec

P = pressure in the diffusion cell

p = partial pressure of the diffusing vapor

A = diffusion tube cross-sectional area (cm^2)

L = Diffusion tube length (cm)

With 3/16-inch ID tubing, A/L was equal to 0.0124 cm. At a temperature of T = 35°C (308 K) and P = 747 torr, $q_d = 5.6 \times 10^{-5}$ ml/sec. At an initial flow rate of 0.25 SLPM, one has a computed concentration of 13.4 ppm. Maximum flow rate was set to 2.1 SLPM yielding a computed concentration of 1.6 ppm.

3.6.2 Experimental Procedures

Once diffusion was initiated, equilibrium was attained in about 24 hours and remained constant for weeks. Internal pressure disturbances above the solution cause only short-termed fluctuations in concentration.

Materials employed in the diffusion generator included a triple necked pyrex distillation flask fitted with $\mathfrak{F}$ 24/40 PTFE stoppers lightly coated with a Hooker Chemical Company fluorolube grease (GR-90), stainless steel fittings and PTFE tubing. Temperature was maintained by an agitated temperature controlled water bath.

3.7 NITRIC ACID (HNO_3) THERMAL CONVERSION

Thermal conversion of HNO_3 as an analytical method for stratospheric monitoring is, as yet, untried. The method, however, has been laboratory tested by D. H. Stedman (private communication, 1977) for tropospheric monitoring and by the authors as discussed in this section. The converter is constructed of glass and contains glass beads for heat transfer. Temperature is maintained at about 550 K. The kinetics of the various reactions of this section relating to HNO_3 have been carefully reviewed. Decomposition of HNO_3 is often heterogeneous, requiring a surface and its formation rate does not lend itself to description by Arrhenius' equation. The function of the surface appears to be to act as an OH scavenger.

3.7.1 Theory

Conversion of HNO_3 has been experimentally treated by Frejacques (1951) and extensively by Johnston et al. (1951, 1953, 1955).

The postulated reaction of Frejacques is the following:

$$2\, HNO_3 \longrightarrow NO + NO_2 + O_2 + H_2O \qquad (24)$$

with N_2O_5 as an intermediary product. Subsequent measurements by colleagues of Johnston and the authors indicate that the thermal conversion follows the Johnston path. The thermal conversion is a complex reaction with the net stoichiometric reaction:

$$4\ HNO_3 \longrightarrow 4NO_2 + 2\ H_2O + O_2 \qquad (25)$$

A consecutive side reaction is the thermal conversion of NO_2 to NO which was treated in Section 3.3.1.1. The ensuing analysis does not consider this side reaction.

In the presence of NO, the thermal conversion is also a complex reaction with the net stoichiometric reaction:

$$2HNO_3 + NO \longrightarrow 3NO_2 + H_2O \qquad (26)$$

This reaction is treated after a discussion of reaction (25).

The governing mechanistic reactions for reaction (25) are the decomposition and recombination of HNO_3 followed by a product-reactant reaction followed by the two N_2O_5 simultaneous bimolecular reaction paths, one of which has a fast-sequential reaction converting NO, if present. These reactions are (H. S. Johnston, 1955):

$$HNO_3 \xrightarrow{[M]} HO + NO_2 \qquad (27)$$

$$HO + NO_2 \xrightarrow{[M]} HNO_3 \qquad (-27)$$

$$HO + HNO_3 \longrightarrow H_2O + NO_3 \qquad (28)$$

$$NO_2 + NO_3 \xrightarrow{k29} NO + NO_2 + O_2 \qquad (19)$$

$$NO + NO_3 \xrightarrow{k30} 2NO_2 \qquad (7)$$

The earlier work of Johnston et al. (1951) indicated that decomposition of HNO_3 was first order for temperatures above 670 K and given approximately as $k_{25} = 1.34 \times 10^9 \exp(-32{,}600/RT)\ s^{-1}$. For temperatures below 570 K, the decomposition proceeded initially as a first-order reaction followed by a rate slower than first-order. Appearance of this transition was also a function of the reaction vessel size.

The later work of Johnston et al. (1955) concerning HNO_3 indicated that for temperatures above 650 K and a 2-liter Vycor bulb, the decomposition of pure HNO_3 followed reaction (25) with a first-order rate constant proportional to initial concentration. The proportionality is an empirical second-order rate constant given by $k_{25} = 9.3 \times 10^{-17} \exp(-38{,}300/RT)$ cm^3-molecule^{-1}-s^{-1}. Using argon and oxygen as foreign gasses in separate experiments, the first-order rate constant was found to be about $5.38 \times 10^4 \left[M\right] + 0.006$ s^{-1} for $\left[M\right] < 2.4 \times 10^{14}$ molecules/cm^3, a temperature of 673 K and initial HNO_3 concentraction of 1.29×10^{14} molecules/cm^3. At temperatures of interest, the second-order rates are

$$k_{25} = 7.3 \times 10^{-35} \text{ cm}^{-3}\text{-molecules}^{-1}\text{-s}^{-1} \quad (298 \text{ K})$$
$$= 5.5 \times 10^{-22} \quad (550 \text{ K})$$

The primary step in all the reactions of HNO_3 bimolecular decomposition is that of reaction (27), the formation of nitrogen dioxide and the hydroxyl radical. At low total pressures (<5 torr) and, therefore, slower rates, nitric oxide and nitrogen dioxide accelerate and inhibit, respectively, the decomposition.

Atkinson et al. (1976) along with others have studied the formation rate of HNO_3, i.e., reaction (-27). The data is summarized in the NASA Reference Publication 1010 (1977). The recommended form for k_{-27} is very complex (Hampson and Garvin 1978) but a reasonable approximation can be found in Anderson et al. (1974). The expression they obtain is:

$$k_{-26} = 2.3 \times 10^{-30} \times (295/T)^{2.5} \text{cm}^6\text{-molecule}^{-1}\text{-s}^{-1}$$
$$295 \leq T \leq 450 \text{ K}$$

The forward decomposition reaction rate, k_{27}, can be derived using the equilibrium constant for the reaction, $K_{27,-27}$

$$K_{27,-27} = (1.3 \times 10^{30}/T \exp\left[-24970/T\right] \text{ molecules-cm}^{-3},$$

where $K_{27,-27}$ has been evaluated at room temperature using the JANAF tables. The functional form of $K_{27,-27}$ should not change appreciably with temperature over the range of interest. Thus, the form for the forward reaction can be found

$$k_{27} = K_{27,-27} \times k_{-27} = (3.0/T)\,(295/T)^{2.5} \exp\left|-24970/T\right| \; cm^3\text{-molecules}^{-1}\text{-s}^{-1}$$

$$k_{27}M = 4.6 \times 10^{-20}\ s^{-1} \qquad (298\ K,\ 1\ atm)$$

$$= 0.36\ s^{-1} \qquad (650\ K,\ 1\ atm)$$

and $k_{-27}M = 6.2 \times 10^{-11}\ cm^3\ \text{-molecule}^{-1}\text{-s}^{-1}$

$$- 8.6 \times 10^{-12}\ cm^3\ \text{-molecule}^{-1}\text{-s}^{-1}\ (650\ K,\ 1\ atm)$$

Similarly, for reaction (28), the forward rate has been evaluated (Hampson and Garvin, 1978),

$$k_{28} = 8 \times 10^{-14}\ cm^3\text{-molecule}^{-1}\ \text{-s}^{-1}\ (240 \le T \le 406\ K).$$

The equilibrium constant, $K_{28,-28}$, derived from the JANAF tables satisfies the equation

$$K_{28,-28} = 2.6 \exp\left[9160/T\right].$$

Thus, the backward reaction rate, k_{-28}, becomes:

$$k_{-28} = (k_{28}/K_{28,-28}) = 2.4 \times 10^{-14} \exp\left|-9160/T\right|\ cm^3\ \text{-molecule}^{-1}\text{-s}^{-1}$$

$$= 2.6 \times 10^{-41}\ cm^3\ \text{-molecule}^{-1}\ \text{-s}^{-1}\ (298\ K)$$

$$= 1.8 \times 10^{-20}\ cm^3\ \text{-molecule}^{-1}\ \text{-s}^{-1}\ (650\ K)$$

For reaction (25) the growth of NO_2 is given by:

$$\frac{d\left[(NO_2)\right]}{dt} = k_{25}\left[HNO_3\right] - k_{25}\left[HO\right]\left[NO_2\right] + 2\,k_{28}\left[NO\right]\left[NO_3\right]. \qquad (3\text{-}32)$$

Noting that HO, NO_3 and NO are the temporary or intermediary molecules and employing successive steady-state approximations until a solution is reached, we consider the rate of change of HO with respect to time first. This is given by;

$$\frac{d\left[HO\right]}{dt} = k_{27}\left[HNO_3\right] - k_{-27}\left[HO\right]\left[NO_2\right] - k_{28}\left[HO\right]\left[HNO_3\right] \qquad (3\text{-}33)$$

Accepting the statement that HO will be short-lived at high temperature, the generation and removal rates will be comparable, so that d $[HO]$/dt will be zero. This is a statement equivalent to the steady-state approximation for kinetic reactions. With this in mind,

$$k_{27} \left[HNO_3\right] = k_{-27} \left[HO\right] \left[NO_2\right] + k_{28} \left[HO\right] \left[HNO_3\right] \quad (3\text{-}34)$$

or that

$$\left[HO\right] = \frac{k_{27} \left[HNO_3\right]}{k_{-27} \left[NO_2\right] + k_{28} \left[HNO_3\right]} \quad (3\text{-}34a)$$

The rate of change or growth of the radical NO_3 is given by;

$$\frac{d\left[NO_3\right]}{dt} = k_{28} \left[HO\right] \left[HNO_3\right] - k_{29} \left[NO_2\right] \left[NO_3\right] - k_{30} \left[NO\right] \left[NO_3\right] \quad (3\text{-}35)$$

Making the same steady-state approximation for NO_3 as with HO, one has;

$$k_{28} \left[HO\right] \left[HNO_3\right] = k_{29} \left[NO_2\right] \left[NO_3\right] + k_{30} \left[NO\right] \left[NO_3\right] \quad (3\text{-}36)$$

or that;

$$\left[NO_3\right] = \frac{k_{17} \left[HO\right] \left[HNO_3\right]}{k_{29} \left[NO_2\right] + k_{30} \left[NO\right]} \quad (3\text{-}36a)$$

Combining equations (3-36a) and (3-34) one has that;

$$k_{27} \left[HNO_3\right] = k_{-27} \left[HO\right] \left[NO_2\right] + k_{29} \left[NO_2\right] \left[NO_3\right] = K_{30} \left[NO\right] \left[NO_3\right] \quad (3\text{-}37)$$

when equations (3-37) and (3-32) are combined, one has after factoring;

$$\frac{d\left[NO_2\right]}{dt} = NO_3 \, (k_{29} \left[NO_2\right] + 3k_{30} \left[NO\right]) \quad (3\text{-}38)$$

From equation (3-36) one has;

$$\left[NO_3\right] = \frac{k_{28}\left[HO\right]\left[HNO_3\right]}{k_{29}\left[NO_2\right] + k_{30}\left[NO\right]} \tag{3-39}$$

or since,

$$\left[HO\right] = \frac{k_{28}\left[HNO_3\right]}{k_{-27}\left[NO_2\right] + k_{28}\left[HNO_3\right]} \tag{3-40}$$

from equation (3-34), NO_3 can be written as,

$$\left[NO_3\right] = \frac{\dfrac{k_{28}k_{27}\left[HNO_3\right]^2}{k_{-27}\left[NO_2\right] + \left[k_{28}\right] HNO_3}}{k\left[NO_2\right] + k_{28}\left[NO\right]} \tag{3-41}$$

The final result desired is obtained by combining equations (3-41) and (3-38) to yield;

$$\frac{d\left[NO_2\right]}{dt} = \frac{k_{28}k_{27}\left[HNO_3\right]^2}{k_{-27}\left[NO_2\right] + k_{28}\left[HNO_3\right]} \times \frac{k_{29}\left[NO_2\right] + 3\,k_{30}\left[NO\right]}{k_{29}\left[NO_2\right] + k_{30}\left[NO\right]} \tag{3-42}$$

which can be simplified, since $k_7 >> k_{29}$ (pg 39), to;

$$\frac{d\left[NO_2\right]}{dt} = \frac{3k_{28}k_{27}\left[HNO_3\right]^2}{k_{-27}\left[NO_2\right] + k_{28}\left[HNO_3\right]} \tag{3-43}$$

For reaction (28) the rate of loss for HNO_3 is given by:

$$-\frac{d\left[HNO_3\right]}{dt} = \frac{2k_{27}k_{28}\left[HNO_3\right]^2}{k_{-27}\left[NO_2\right] + k_{28}\left[HNO_3\right]} \tag{3-44}$$

With NO present, one has the following net stoichiometric reaction:

$$2HNO_3 + NO \longrightarrow 3NO_2 + H_2O \tag{26}$$

so that the final concentration of NO_2 is 1.5 times that of the HNO_3. For low pressure Johnston et al. (1955) has postulated that five steps are required. The governing mechanistic reactions for reaction (26) are the decomposition of HNO_3 followed by a product-reactant reaction followed by a fast

bimolecular reaction converting NO to NO_2 followed by the synthesis of nitrous acid as an intermediary and finally a reaction to consume the nitrous acid. These reactions are:

$$HNO_3 \xrightarrow{[M]} HO + NO_2 \tag{27}$$

$$HO + HNO_3 \longrightarrow H_2O + NO_3 \tag{28}$$

$$NO + NO_3 \longrightarrow 2NO_2 \tag{7}$$

$$NO + NO_2 + H_2O \longrightarrow 2HNO_2 \tag{29}$$

$$HNO_2 + HNO_3 \longrightarrow 2NO_2 + H_2O \tag{30}$$

3.7.2 Stratospheric-Based Instrument Modeling

The above set of reactions along with the N_2O_5 set of reactions given in paragraph 3.5.1 have been modeled using the EPISODE code to analyze and review concentration-time profiles of the various molecules and radicals. For laboratory conditions the profiles indicate that OH scavenging and elevated temperature promote the decomposition of HNO_3. For stratospheric conditions the profiles (c.f., Appendix B-2) indicate that only increased temperature promotes the decomposition of HNO_3, i.e., the intermediary radical, OH does not impede decomposition.

3.7.3 Experimental Procedures and Results

The thermal decomposition of nitric acid was investigated in the laboratory with emphasis placed on a quantitative understanding and investigation of the thermal converter. In addition, ozone was introduced into the HNO_3 vapor stream to determine whether it had an effect on the thermal conversion process.

The thermal converter based on a design by Stedman (private communication, 1977), consisted of 40 cm long by 1/2-inch O.D. stainless steel tubing, packed with 1/8-inch diameter Pyrex balls. (The Pyrex balls served to raise the temperature of the gas to that of the tubing.) The tubing was wrapped with electrical heating tape and placed in an insulated cylinder. The temperature of the tubing, which could be raised as high as 500°C, was monitored

by a thermocouple inserted into the gas stream exiting the converter. The temperature could also be monitored by observing the $[NO_2]/[NO]$ ratio of the exiting gas stream when NO_2/air was passed through the converter.

The gas leaving the thermal converter was directed into an absorption cell, placed within a Perkin-Elmer Model 580A spectrophotometer. The internal optics of the absorption cell were set to an optical absorption path length of 15.75 m. The infrared absorption properties of HNO_3, NO_2, and O_3 are discussed in Appendix A of this report. By combining the known optical properties of these molecules with the observed IR absorptions, the number density of each specie was determined.

From the absorption cell, the flowing gas was directed to the Aerochem chemiluminescence monitor. The monitor was primarily used to detect NO (whose IR absorption signature is especially weak) and to verify the spectroscopically determined, NO_2 concentrations. A comparison of the analytical methods using the CL monitor as opposed to those of the spectrophotometer was made by using an NO_2/air span gas diluted by additional nitrogen to maintain a constant flow rate (Figure 3-12). Agreement between the two instruments was quite good. The CL monitor response also was determined as a function of gas flow rate (Figure 3-13). Since the CL monitor has a constant volume bellows pump within it to draw in the gas sample, the pressure in the sample line will vary as the flow rate is externally controlled, but the response remains proportional to the flow rate.

It was shown in paragraph 3.6.1 that the concentration of HNO_3 depended inversely on the gas flow rate. Therefore, to vary the concentration of HNO_3, the flow rate was varied. However, pressure in the absorption cell was maintained at constant value by adjusting a throttle valve located at the exit port of the cell. CL monitor readings were "normalized" to take into account the varying flow rate.

The results of a set of measurements of the thermal conversion of HNO_3 are given in Table 3-16. The absorption data is based on the average of three or more successive spectra recorded after equilibrium was established. The standard deviation of the data is also shown. The CL monitor response for

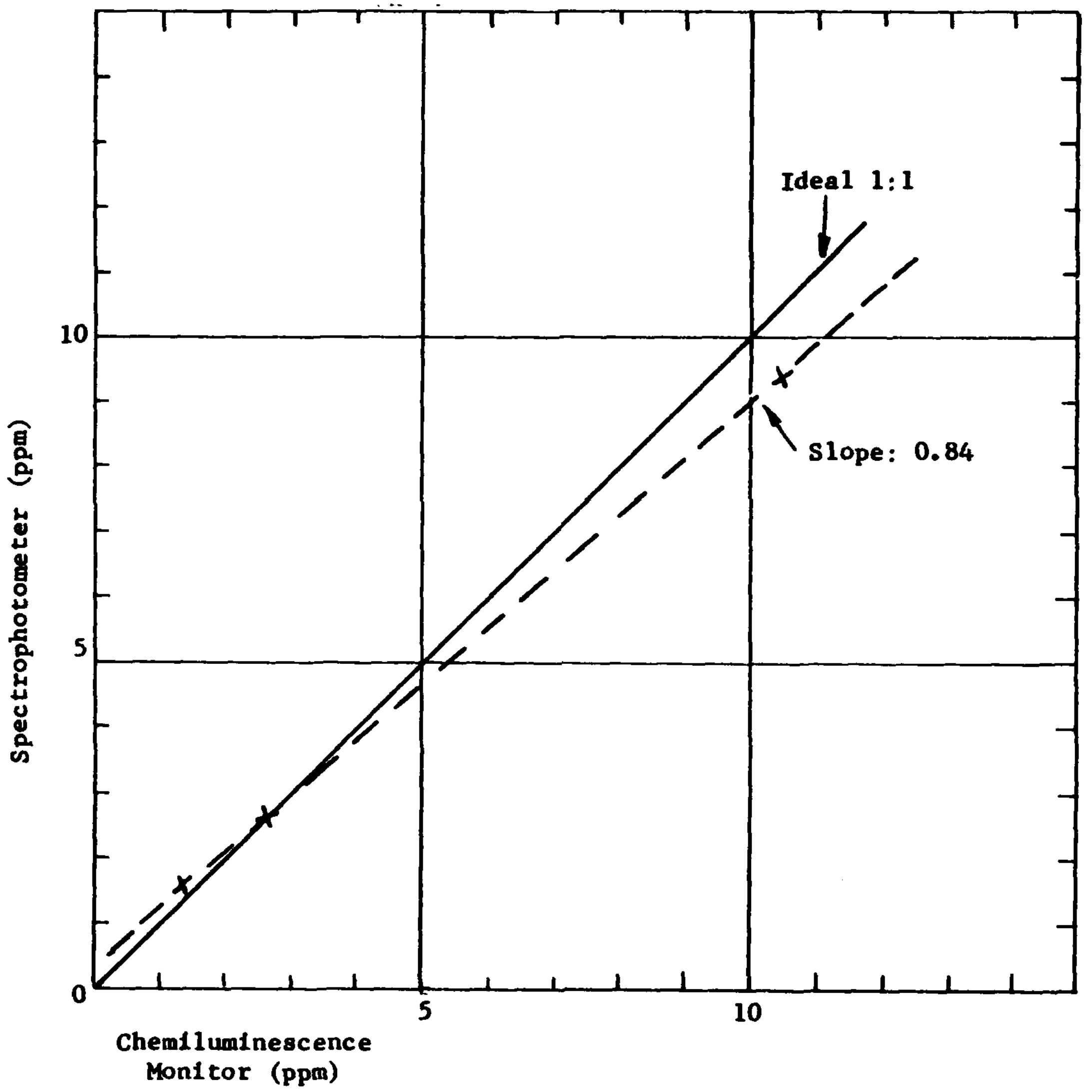


Figure 3-12. Response of Perkin-Elmer Model 580 Spectrophotometer vs. Chemiluminescence Monitor

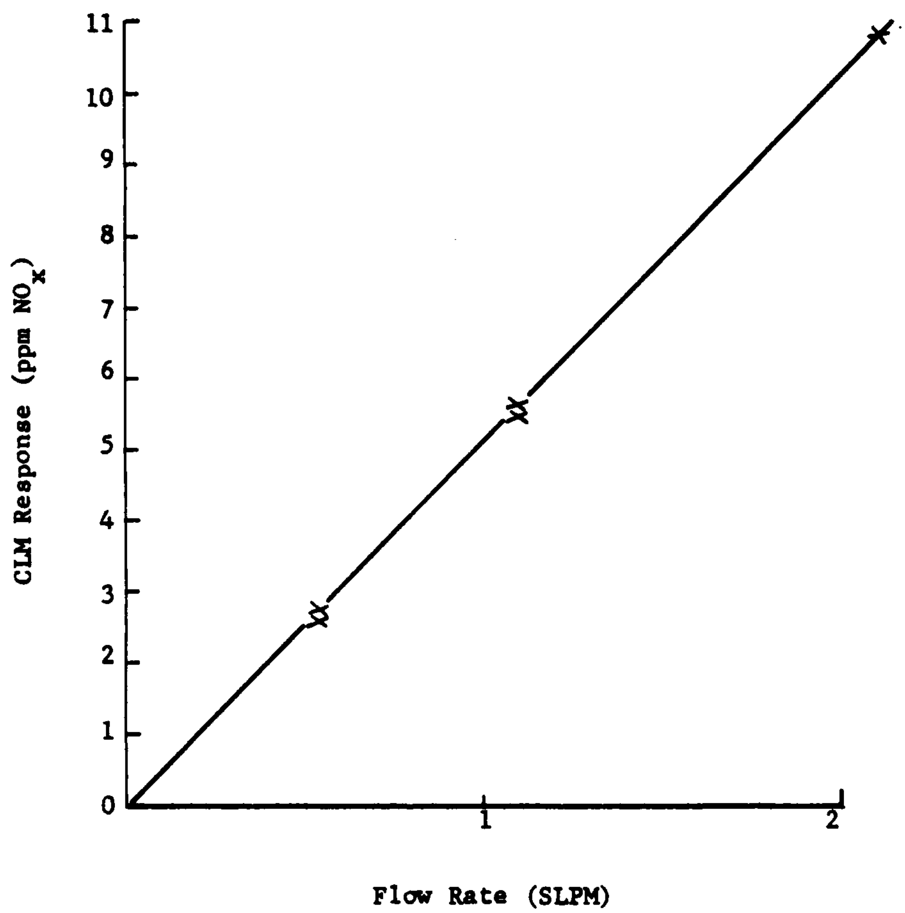


Figure 3-13. Chemiluminescence Monitor Performance vs. Flow Rate

TABLE 3-16. HNO_3 THERMAL CONVERTER[a] PERFORMANCE CHARACTERISTICS WITH CROSS CALIBRATION HIGH TEMPERATURE CATALYTIC CONVERSION VS CHEMILUMINESCENCE MEASUREMENTS

Apparatus	Sampling Point	Concentration	Analysis Techniques
Low Temperature Converter, T = 535 $\pm$ K	Inlet	$[HNO_3] = 7.2 \pm 0.4$ ppm	IR Absorption
	Outlet	$[NO_2] = 7.1 \pm 0.4$ ppm	IR Absorption
		$[NO_2] = 7.8$ ppm	Thermal-CLM
		$[NO] = 0.6$ ppm	CLM
		$[NO_2]/[NO] = 14.0$[b]	Ratio
High Temperature Catalytic Converter and CLM	Inlet	$[HNO_3] = 7.2 \pm 0.4$ ppm	IR Absorption
	Outlet Sample	"$[NO_2]$" = 7.7	Thermal-CLM

[a] Tubular Pyrex Converter with 3 mm Pyrex Spheres

[b] Equivalent to Thermodynamic Conversion Ratio Expected for T = 535 K

the NO_x mode was scaled to compensate for the changing flow rate. The NO and NO_x-NO density data were derived from the NO_x data and from NO concentration data which was also recorded by the monitor.

Comparison of the second and third lines of the table shows that the amount of NO (from the CL monitor) plus NO_2 (from the spectrophotometer) is approximately 7.6×10^{13} molecules/cm^3, which is very good agreement. It is also apparent by comparing lines 3 and 4 that the Aerochem instrument responds accurately to HNO_3 vapor. Comparison of the CL monitor with the Model 580A (Figure 3-12) indicated a 5 to 15 percent disagreement. This uncertainty limits our ability to compare data to an accuracy of no more than 10 percent. Finally, the $[NO_2]/[NO]$ ratio indicates a gas temperature in the 520 to 550 K range.* The equilibrium constant, $K_{25,-25}$, at this temperature indicates that the HNO_3 should be entirely decomposed.

In an earlier experiment, dry nitrogen rather than air was used as the carrier gas for the HNO_3 vapor. The products of the decomposition were NO_2 and NO, with their ratio being $[NO_2]/[NO] = 3.48 \pm 0.91$; the HNO_3 concentration was 5.68×10^{13} molecules/cm^3. The optically detected NO_2 density was 4.52×10^{13}. Taking into account the measured ratio of $[NO_2]$ to $[NO]$, the sum of $[NO]$ and $[NO_2]$ was 5.82×10^{13} molecules/cm^3 which is, again, very close to the original HNO_3 number density. The uncertainty associated with these measurements was on the order of ± 10 percent. The reason the $[NO_2]$ to $[NO]$ ratio differed from the data discussed previously is related to the use of nitrogen. The NO_2 decomposition reaction to form NO has been discussed (paragraph 3.3.1.1); the equilibrium constant is independent of the carrier gas (air or nitrogen) while the actual ratio of $[NO_2]$ to $[NO]$ is not. This explains the difference in the ratio for the two cases. For either carrier gas, the thermal decomposition of HNO_3 was total to within experimental error. The maximum flow rate used was 2.1 SLPM.

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*For determination of the $[NO_2]/[NO]$ ratio, the following expression has been used;

$$\log \frac{[NO_2]}{[NO]} = \frac{3002}{T} - 4.223 \qquad (3\text{-}15)$$

and is applicable at standard pressure and $pO_2 = 152$ torr.

3.8 POTENTIAL INTERFERENTS (Specificity)

Potential interferents that could affect the performance of a hybrid chemical conversion system include members of both the ClO_xNO_x family of compounds and the HO_xNO_x family of compounds. These potential interferents would effect the performance through either photolytic effects or thermal lability effects. This program has (1) analyzed photolytic effects of the ClO_xNO_x compounds, (2) experimentally treated $ClONO_2$ until accidental loss of all material occurred, and (3) analyzed thermal lability effects of $ClONO_2$ and HO_2NO_2.

3.8.1 ClO_xNO_x Family Compounds

This section treats the potential interference of nitrosyl chloride (ClNO), nitryl chloride, chlorine nitrite (ClONO), and chlorine nitrate ($ClONO_2$) with particular emphasis on $ClONO_2$ since it is believed to be the most predominant member of the ClO_xNO_x family with the stratosphere.

3.8.1.1 $ClONO_2$ Generation and Handling

Chlorine nitrate has been synthesized by three methods. The first method (M. Schmeisser, 1963) is based upon the reaction:

$$Cl_2O + N_2O_5 \longrightarrow ClONO_2 \qquad (31)$$

The boiling point of nitrate is about 18 to 22°C and the melting point about -107°C. Decomposition occurs slowly at room temperature, but since Cl_2O is very sensitive to heat, $ClONO_2$ is commonly stored at -78°C or at 77 K. For research quantities, much of the $ClONO_2$ used in the United States has been generated and distributed by Dr. Louis C. Glasgow of E.I. DuPont de Nemours and Company. Containerization employs glass ampules or 1 liter stainless steel sampling cylinders.

A second method (Birks et al., 1977) is based upon the reaction:

$$ClO + NO_2 + N_2 \longrightarrow ClONO_2 + N_2 \qquad (32)$$

The initial reactants employed are 0.25 percent Cl_2 in He, O_2 for the generation of O_3 and NO_2 in air. Two mixing stations are required; the first

downstream from a microwave cavity, which is used for generating atomic chlorine, and an ozonator. The second is downstream for the ClO and NO_2 sources.

The third method (Schack, 1967) is based upon the reaction:

$$ClF + HNO_3 \longrightarrow ClONO_2 + HF \quad (33)$$

The technique avoids the use of hazardous chlorine oxides since the initial reactants are separately condensed at 77 K into a stainless steel container. Bulb to bulb cryogenic vacuum distillation separates the $ClONO_2$ from the hydrofluoric acid.

The $ClONO_2$ used for this program was generated by Dr. Glasgow, on February 3, 1977, using the first method. The batch (about 5 gms material at 77 K) underwent four bulb to bulb distillations before delivery and a fifth distillation to remove further accumulated impurities was carried out at Perkin-Elmer on September 12, 1978. The material was held at 77 K between the last two distillations. Impurities generally include Cl_2, NO_2, N_2O_5, HNO_3, and possibly ClO_2. Absorption spectra in the UV region indicated that the transfered batch contained substantial Cl_2, but no discernible NO_2.

The vapor pressure of $ClONO_2$ is given by the expression (Schack, 1967):

$$\log P = \frac{-0.05223\ A}{T} + B\ \text{(torr)}$$

where A = 28,900 and B = 7.9892. This expression versus 1000/T is shown in Figure 3-14 along with similar data from International Critical Tables for the possible impurities Cl_2, NO_2, N_2O_5, and HNO_3. For the fifth distillation, Cl_2 was pumped off at 163 K using a slush of methyl butane (isopentane) and liquid nitrogen. The batch was then elevated in temperature to about 223 K and the $ClONO_2$ was allowed to enter an IR absorption cell at a pressure of about 14 torr or condensed in a one-liter stainless steel container.

Materials in contact with the sample included glass, teflon,®*, stainless steel, KBr and halofluorocarbon grease, GR-90.

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*PTFE, Polytrifluoromonochloroethylene

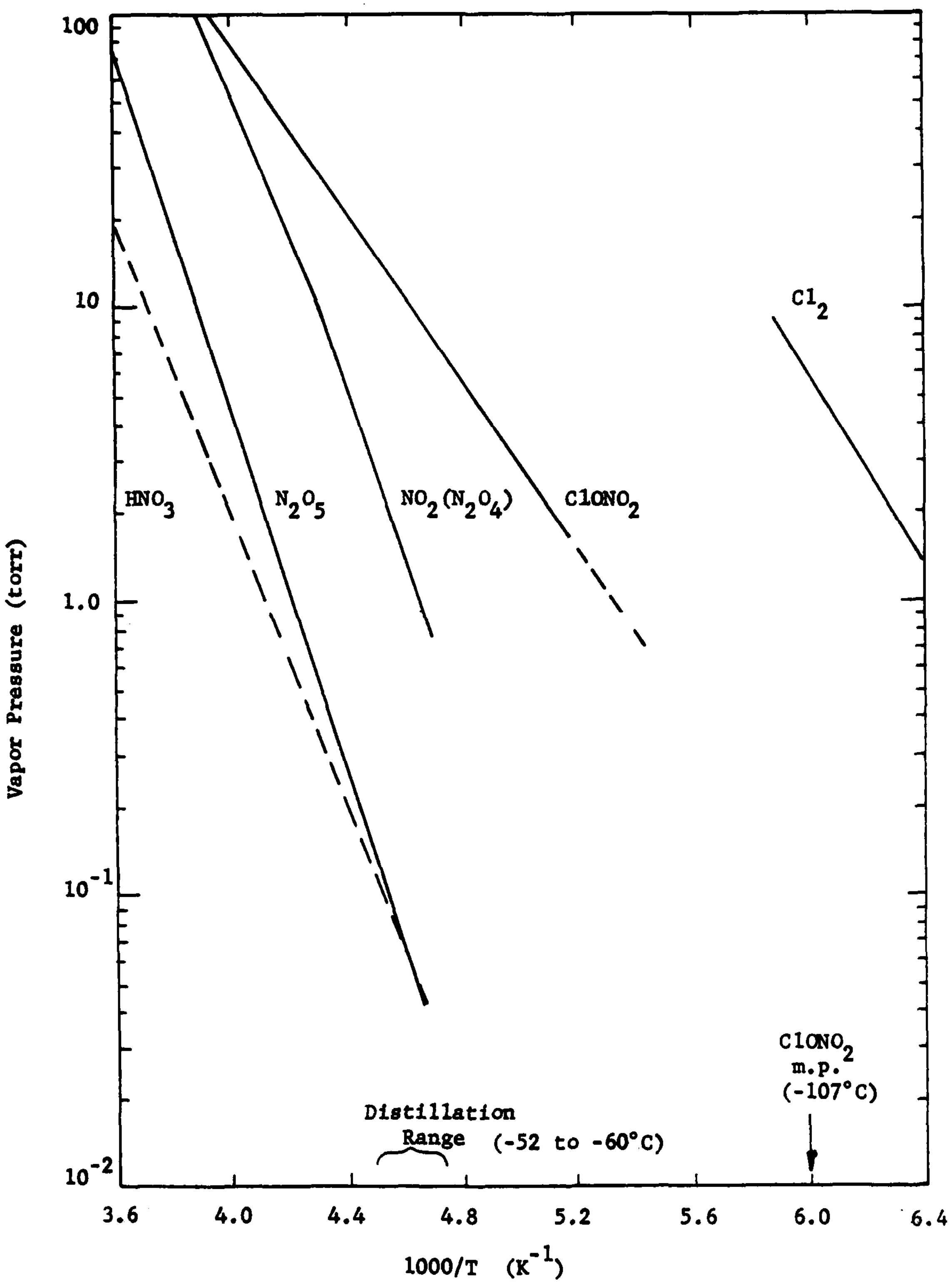


Figure 3-14. Vapor Pressure Diagram For $ClONO_2$ and Suspected Impurities

The $ClONO_2$ absorbance was then measured on a Perkin-Elmer Model 521 spectrometer using a preset resolution of 3 cm^{-1} for survey over the region 1800 to 650 cm^{-1}. During transfer of the cell to the spectrometer, the sample was held at about 273 K and protected from room lighting by Wratten-type filter material.

Two lengthy survey scans were performed and analyzed as the $ClONO_2$ thermally decomposed at a temperature close to 306 K. The decay of $ClONO_2$ is shown in Figure 3-15 and a summary of the data is given in Table 3-17. Due to the large absorbance of $ClONO_2$, the initial fill pressure of about 14 torr was reduced to a pressure of about 4.5 torr. The unused portion of $ClONO_2$ was diluted with nitrogen and stored at LN_2 temperature for later use. Failure of the automatic LN_2 transfer system during an unattended period caused the $ClONO_2$ to attain room temperature with a subsequent thermal decay.

3.8.1.2 ClO_xNO_x Photolytic Interferents

It is possible that, should an NO_2 photolytic converter be used prior to chemiluminescence of NO with O_3, the ClNO, $ClNO_2$, ClONO, and $ClONO_2$ will be photolyzed to yield a higher reading of NO_2. This possibility is not considered to be significant as is shown below, where what is believed to be typical concentration levels and a white-light photolytic source appropriately filtered with Corning C.S. 7-54 and 320-nm glass filters are assumed.

Although three members of the ClO_xNO_x family are not considered among the "most important" trace species of the stratosphere and, therefore, have received very little attention, they do have significant near-UV absorption cross-sections as is seen shown in Figure 3-16. The fourth species, $ClONO_2$ is considered to be an important sink as it does not appear to react with O_3 and reacts only slowly with O.

By employing Corning C.S. 7-54 and 320-nm filters, an NO_2 photolytic technique was developed that rendered NO_3 a negligible interferent. The same analysis was applied to the ClO_xNO_x family to test the specificity of the technique. The results of the analysis are shown below in Table 3-18 with the appropriate absorption cross-sections taken from Figure 3-16.

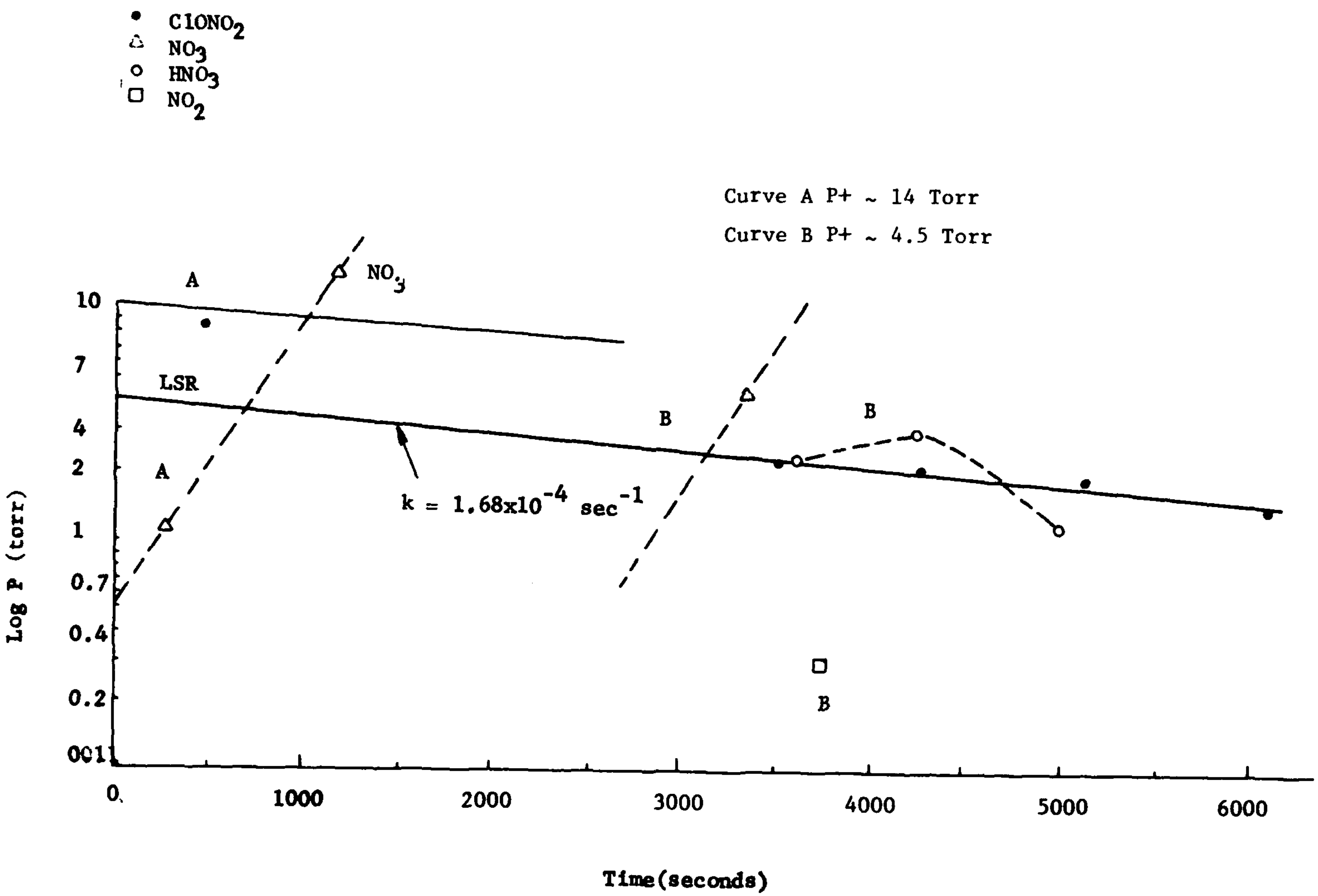
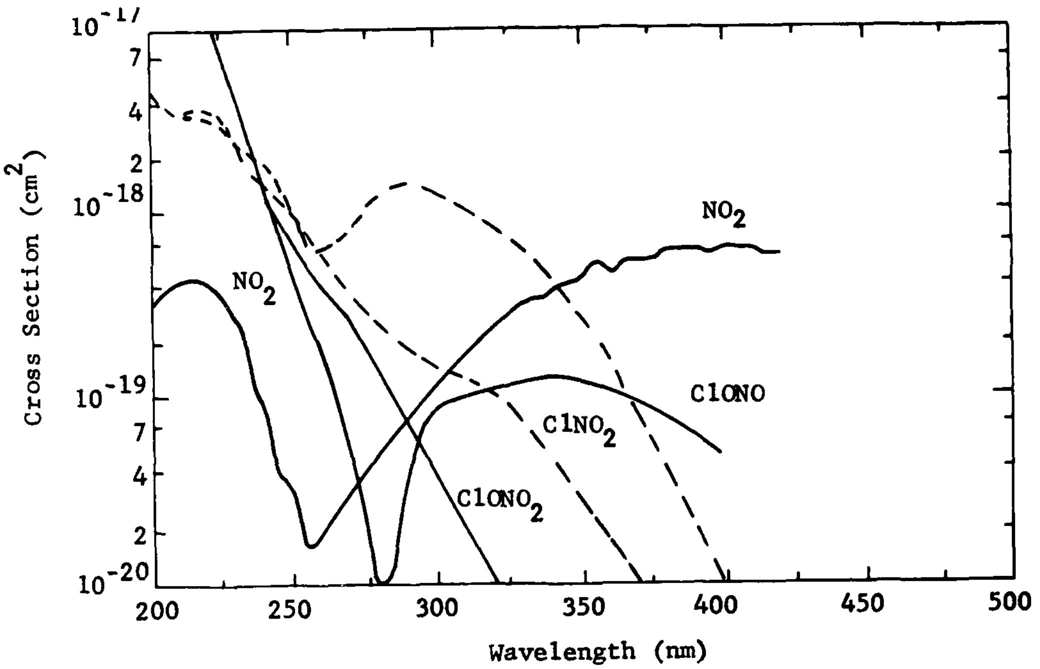


Figure 3-15. Thermal Decomposition of $CLONO_2$, T ~ 306 K

TABLE 3-17. $ClONO_2$ THERMAL DECOMPOSITION

Time (Sec)	Species	Analytical Band (cm^{-1})	Number Density ($Molec/cm^3$)	Partial Pressure (Torr)	Total Pressure
285	NO_3	1860	0.04×10^{18}	1.13	~14 Torr
480	$ClONO_2$	(ν_1)1735	0.27	8.5	
1160	NO_3	1345	0.48	15	
1250	$ClONO_2$	(ν_2)1292	0.34	10.6	
1335	N_2O_5	(ν_{12})1246	0.0049	0.154	
3330	NO_3	1860	0.14	4.29	~4.5 Torr
3520	$ClONO_2$	(ν_1)1735	0.068	2.14	
3580	HNO_3	(ν_2)1706	0.071	2.22	
3760	NO_2	(ν_3)1600	0.0091	0.29	
4280	HNO_3	(ν_4)1311	0.095	2.98	
4290	$ClONO_2$	(ν_2) 1292 (1288)	0.064	2.03	
4970	HNO_3	890	0.037	1.17	
5140	$ClONO_2$	(ν_4) 780	0.056	1.77	
6090	$ClONO_2$	(ν_1)1735	0.044	1.39	



NO_2 Curve Adapted from H.S. Johnston and R. Graham, Can. J. Chem 52, 1415 (1974). Other Curves from NASA Reference Publ. 1010, Chlorofluoromethanes and the Stratosphere, edited by R. Hudson, Aug 1977

Figure 3-16. NO_2 and ClO_xNO_x Absorption Cross-Sections

TABLE 3-18. ClO_xNO_x-NO_2 PHOTOLYSIS SPECIFICITY WITH SPECTRAL DISCRIMINATION

Species	$\sum_{300}^{420} \sigma\lambda_s \tau_\lambda \, d\lambda \times 10^{19} cm^2$-nm	$\sum_{300}^{420} \sigma\lambda_s \tau_\lambda d\lambda$ $\sum_{300}^{420} \sigma_{NO_2} \tau_\lambda d\lambda$
Nitrogen dioxide, NO_2	278	1.00
Nitrosyl chloride, ClNO	74	0.27
Nitryl chloride, $ClNO_2$	25.2	0.091
Chlorine nitrite, ClONO	289	1.04
Chlorine nitrate, $ClONO_2$	2.7	0.01

Almost nothing is known about the stratospheric concentrations or mixing ratios of the ClO_xNO_x species cited above. Modeling efforts to date extend only to $ClONO_2$ (F.M. Luther, 1976; and NAS, 1976), and an upper limit of 2 ppb using the limb sensing techniques has been set (D.G. Murcray et al., 1977).

At stratospheric altitudes chlorine nitrate is produced at night by the combination of the radial ClO with NO_2 according to

$$ClO + NO_2 + N_2 \rightarrow ClONO_2 + N_2 \qquad (32)$$

During periods of high insolution, $ClONO_2$ is photolyzed via

$$ClONO_2 + h\nu \rightarrow ClO + NO_2 \qquad (34a)$$

$$\rightarrow Cl + NO_3 \qquad (34b)$$

At high altitude, i.e. $H > 40$ km, the photolysis takes place over the 200 to 220 nm spectral region, where the absorption cross-section is $\sim 375 \times 10^{-20}$ cm^2/molecule. At lower altitudes, 20 to 30 km, the diurnal change is much less, with photolysis occurring with radiation greater than 300 nm.

The number density profile of NO_2 and $ClONO_2$ are shown below in Table 3-19. The $ClONO_2$ concentrations are taken from F.M. Luther (1976). As the chlorine nitrate density is well below that of NO_2, the 0.01 of Table 3-18 is further reduced. $ClONO_2$ photolyization is not considered to be a significant problem.

TABLE 3-19. NO_2 AND $ClONO_2$ CONCENTRATIONS

H (km)	NO_2 (30 N) (molecules/cm^3)	$ClONO_2$ (midnight) (molecules/cm^3)	$ClONO_2$ (noon) (molecules/cm^3)
20	1.3×10^9	1.0×10^8	8.0×10^7
25	2.2	4.0	3.0×10^8
30	2.2	1.8	1.0
35	1.4	5.0×10^7	1.0×10^7

3.8.1.3 $ClONO_2$ Thermal Lability

The thermal lability of $ClONO_2$ can impact laboratory handling of the material as well as the specificity of a chemical conversion system that relies on thermal converters. A study by Cox et al. (1977), which employed enthalpy data for $ClONO_2$, led to a high pressure limiting rate given by 10^{14} exp $(-12480/T)$ s^{-1} for the decomposition of $ClONO_2$. This rate is about 3500 times slower than the data of Knauth cited below. The most recent work concerning $ClONO_2$ kinetics is that of H.D. Knauth (1978). Thermal decompositions were studied in the presence of NO, ClNO, and N_2 over the temperature range 303 to 363 K at pressures from 3 to 380 torr.

The unimolecular dissociation of $ClONO_2$ given by:

$$ClONO_2 + (M) \longrightarrow ClO + NO_2 + (M) \qquad (-32)$$

is followed by the fast reaction:

$$NO + ClO \longrightarrow NO_2 + Cl \qquad (35)$$

and chlorine consuming steps.

For pN_2 less than 220 torr, an empirical first-order linear relationship between k_{-32} and $[N_2]$, $k_{-32} = k_{-32a} + k''_{-32}[N_2]$, was determined and suggests that the reaction takes place in the low pressure region or that the departures from the low pressure region are quite small. The rates are given as:

$$k_{-32a} = 2.743 \times 10^{6} \exp(-3350/RT) \ \text{sec}^{-1} \text{ and}$$
$$k''_{-32} = 1.318 \times 10^{-5} \exp(6030/RT) \ \text{cm}^3\text{-mole}^{-1}\text{-sec}^{-1}$$

The Knauth data for $T \geq 333$ K is shown in Figure 3-17 in log-log form. The data for $T \leq 300$ K has been extrapolated from the higher temperature data. The solid square points ($T = 263$ K) correspond to reasonable N_2 diluent storage conditions, but half-life values of only 257 and 82 minutes (at the knee) result. At a temperature of -78°C, the half-line becomes 1.7×10^{8} sec, or 2×10^{3} days.

$ClONO_2 + N_2 \longrightarrow ClO + NO_2 + N_2$

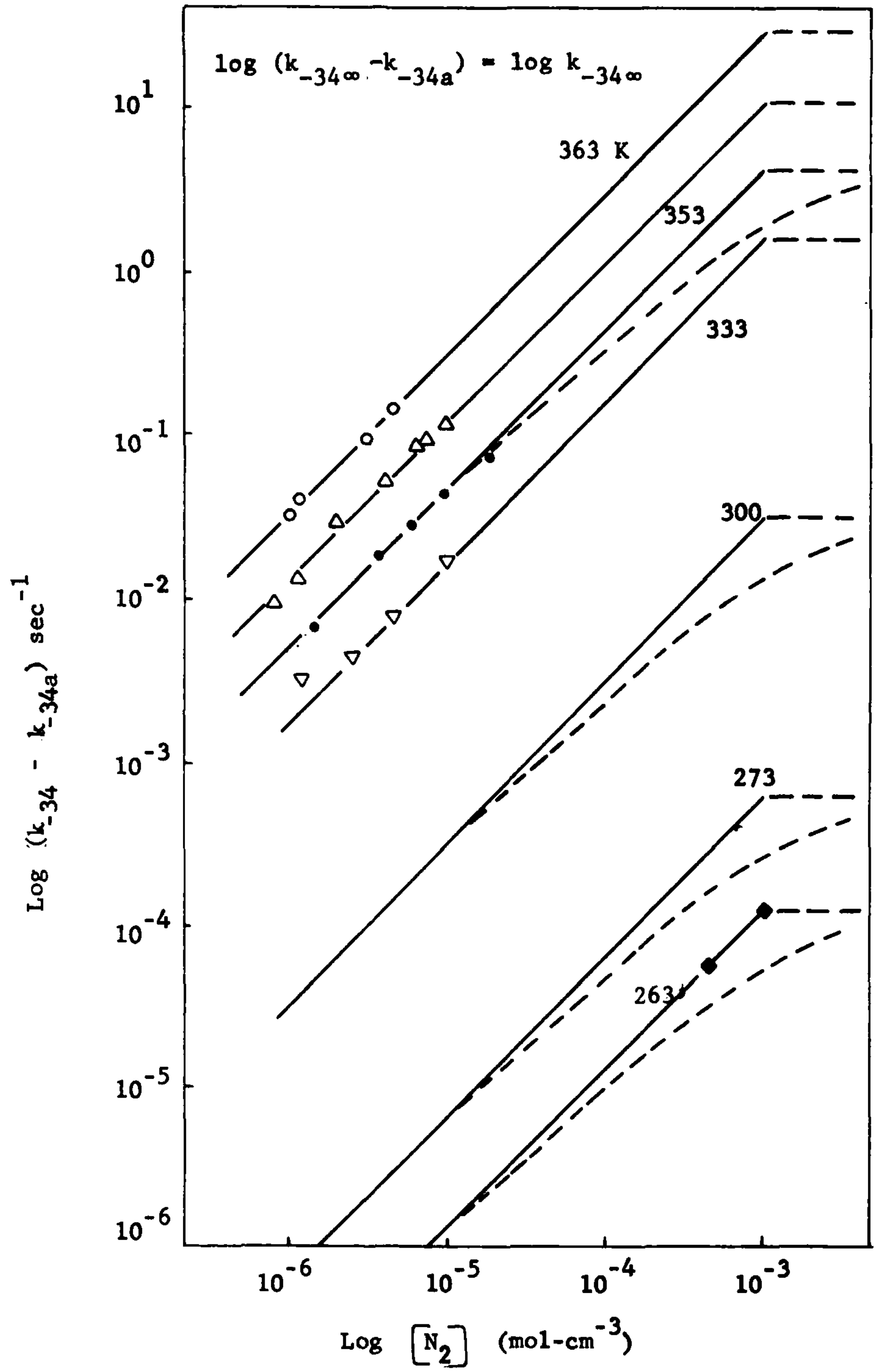


Figure 3-17. Chlorine Nitrate-Nitrogen Dissociation Rates

For the region of the stratosphere of interest $(N_2) \sim 3 \times 10^{18}$ molecules-cm^{-3} and less, so that a 300 K monitoring system with a sample residence time of several seconds would not cause appreciable thermal decay of $ClONO_2$. On the other hand, a 400 K converter for N_2O_5 would result in a $ClONO_2$ half-life of about 0.2 second, causing a lack of specificity for N_2O_5 conversion. Impact on the HNO_3 conversion accuracy due to the relative concentrations would be minimal.

The reaction of NO + $ClONO_2$ leading to an intermediate product but ultimately to ClNO and NO_2 or

$$ClONO_2 + 2NO \longrightarrow ClNO + 2NO_2 \qquad (36)$$

was also studied by Knauth. The rate was found to be 2.09×10^{-12} exp (-11,850/RT) cm^3-molecule^{-1}-s^{-1} over the 303 to 343 K temperature range. At 300 K, Knauth's value of 4.8×10^{-21} cm^3-molecule^{-1}-s^{-1} is in general agreement with that of Rowland et al. (1976). At 800K, the highest anticipated temperature for any of the converters, the rate is still small, 1.2×10^{-15} cm^3-molecule^{-1}-s^{-1}, so NO will not be consumed by the $ClONO_2$. However, the ClO product from thermal decomposition will consume NO.

3.8.2 HO_xNO_x Family Compounds

This section treats the potential interference of nitrous acid (HONO) and pernitric acid (HO_2NO_2); nitric acid ($HONO_2$) having been treated in Section 3.4. Concern with HONO is dismissed by review of pertinent reactions for its generation and high degree of photodissociation during daylight hours. Concern with HO_2NO_2 is not dismissed.

3.8.2.1 Nitrous Acid (HONO)

Nitrous acid is not expected to be an interferent for reasons cited below. It can be formed by four methods. These reactions are:

$$NO + NO_2 + H_2O \rightleftharpoons 2HONO \qquad (29)$$

$$N_2O_3 + H_2O \longrightarrow 2HONO \qquad (36)$$

$$HO_2 + NO_2 \longrightarrow HONO + O_2 \qquad (37a)$$

$$\longrightarrow HO_2NO_2 \qquad (37b)$$

$$N_2O_2 + NO \longrightarrow HONO + HO \qquad (38)$$

Reaction 31 is favored within power plant stacks and near automobile exhausts. Room temperature kinetic studies have been carried out by Chan et al. (1976). Rate constant estimates that use 0.5 cm^{-1} spectroscopy to follow the kinetics are $k_{31} = 6 \times 10^{-38}$ cm^6-$molecule^{-2}$-s^{-1} and $k_{-29} = 9.4 \times 10^{-19}$ cm^3-$molecule^{-1}$-s^{-1}. Since this is a third-order rate equation, it will not proceed to the right unless the conditions are very favorable. Furthermore, if HONO is formed it will be photolyzed with $J > 0$, since $\sigma > 1 \times 10^{-19}$ cm^2/molecule for $340 \leq \lambda \leq 384$ nm (NASA Publ. 1010). Hydridizing nitrogen sesquioxide, reaction 38, has not received much attention. The free radical HO_2 combination with NO_2, reaction 39, favors the formation of HO_2NO_2 since k_{37a}/k_{37b} is about 10^{-3} (Graham et al., 1977). The kinetics of this reaction have also been studied by Simonaitis and Heicklen, (1974).

3.8.2.2 Pernitric Acid (HO_2NO_2)

The formation of HO_2NO_2 via a two-body or three-body mechanism proceeds well enough that it has been modeled by Jesson et al. (1977) with peak concentrations occurring in the 1- to 3-ppb range. It is therefore considered to be a potential interferent.

The reaction kinetics of HO_2 and NO_2 have been studied recently by a number of investigators: Simonaitis and Heicklen (1974, 1976, and 1977), Howard and Evenson (1977), Niki et al. (1977), Jesson et al. (1977), Graham et al. (1977) and Graham et al. (1978). The reactions most often considered are:

$$HO_2 + NO \longrightarrow HO + NO_2 \qquad (39a)$$

$$\longrightarrow HONO_2 \qquad (39b)$$

$$HO_2 + NO_2 \longrightarrow HONO + O_2 \qquad (37a)$$

$$\rightleftharpoons HO_2NO_2 \qquad (37b,-37b)$$

$$2HO_2 \longrightarrow H_2O_2 + O_2 \qquad (40)$$

$$HO_2NO_2 \longrightarrow HONO + O_2 \qquad (41)$$

Reactions (39a) and (39b) are occasionally written as a three-body reaction. The rate constants are given in Table 3-20 in the usual Arrhenius' form. The disparity in term values for k_{-37} will be shown below to have little significance for temperatures greater than 298 K.

As the thermal conversion technique is being considered for N_2O_5 and HNO_3 species, the above cited first-order rates for reaction (-39b) have been developed for laboratory ambient temperature, 400 K and 550 K. These rates, half-lives, and NO_2 concentrations are presented in Table 3-21 for resident times of 1, 2, and 5 seconds. For temperatures above 298 K, conversion is complete in less than a second and yields NO_2. This conversion reduces the specificity of N_2O_5 and HNO_3 measurements. For an NO_2 measurement at an instrument temperature of 298 K, lack of specificity is also present, but to a lesser degree. Straightforward solution to this problem, if the published rates have been correctly extrapolated, is not apparent at this time.

Finally, since the thermal decomposition of HO_2NO_2 changes from first order to second order with reduced pressure, k_{-37b} should be investigated at stratospheric temperatures and pressures $760 >> p > 7$ torr.

3.9 NO_z FEASIBILITY*

For a selective hybrid chemical conversion (SMS), thermal partitioning of thermally labile molecules, N_2O_5 and HNO_3, has led to ambiguous results and therefore such a system is not recommended. The method is also particularly susceptible to interfering species as mentioned in Paragraph 3.8. A non-selective or total odd nitrogen SMS, however, is feasible and described below.

---

*NO_z is defined to be the sum of NO, NO_2, N_2O_5, HNO_3, $ClONO_2$, and HO_2NO_2. Adsorbed NO_z on particulate matter is not specifically treated in the text. Three modes of sampling are believed to be possible. First by using a fluoropore-type filter only, a gas phase sample will be accepted. Second, by employing no filter, both gas phase and adsorbed NO_z will be accepted. A third conceivable mode would be a time shared combination of the first two modes.

TABLE 3-20. HO_xNO_x REACTION RATES

Reaction	Rate (cm^3-$molecule^{-1}$-s^{-1})	Rate (295-300 K) (cm^3-$molecule^{-1}$-s^{-1})	Reference
(41a)	$1.2x10^{-11}$ exp $\left[-(1400+500)/RT\right]$	$1.14x10^{-12}$	Simonaitis and Heicklen (1977)
	$3.0x10^{-11}$exp (-775/RT)	$8.03x10^{-12}$	Howard and Evenson (1977)
(41b)		$2.0x10^{-15}$	Simonaitis and Heicklen (1976)
		$4.5x10^{-30}$	Howard and Evenson (1977)
(39a)	$1.7x10^{-12}$ exp (-1400/RT)	$1.63x10^{-13}$	Simonaitis and Heicklen (1977)
(39b)	Temperature Independent	$4.2x10^{-13}$	Simonaitis and Heicklen (1977)
		$1.97x10^{-31}cm^6$	Howard and Evenson (1977)
(-39b)	$6x10^{17}$ exp (-26000/RT) s^{-1}	$5.16x10^{-2}$ s^{-1}	Simonaitis and Heicklen (1977)
	$1.4x10^{14}$ exp (-20700/RT) s^{-1}	$9.04x10^{-2}$ s^{-1}	Graham et al, (1978)
	$5.2x10^{-6}$ exp (-19,900/RT)	$1.30x10^{-20}$	Graham et al, (1978)
(42)	Temperature Independent	$3.3x10^{-12}$	Simonaitis and Heicklen (1977)
(43)	$1x10^8$ exp (-14000/RT) s^{-1}	$5.4x10^{-3}$ s^{-1}	Simonaitis and Heicklen (1977)

TABLE 3-21. FIRST-ORDER HO_2NO_2 RATE CONSTANTS AND PREDICTED THERMALLY YIELDED NO_2 AS A FUNCTION OF SAMPLE RESIDENCE TIME [a]

	Simonaitis and Heicklen Decay Rate				Graham et al., Decay Rate			
T (K)	k_{-39b} (s-1)	-39b (s)	t_R (s)	NO_2[a] (ppb)	k_{-39b} (s^{-1})	-39b (s)	t_R (s)	NO_2[a] (ppb)
220	8.86×10^{9}	7.8×10^{7}	-	-	3.76×10^{-7}	1.84×10^{6}	-	-
298	5.16×10^{-2}	13.43	1	0.10	9.04×10^{-2}	7.66	1	0.18
			2	0.20			2	0.13
			5	0.45			5	0.72
400	3.80×10^{3}	1.8×10^{-4}	1	2	6.75×10^{2}	1.03×10^{-3}	1	2
			2	2			2	2
			5	2			5	2
550	2.79×10^{7}	2.5×10^{-8}	1	2	8.20×10^{5}	8.45×10^{-7}	1	2
			2	2			2	2
			5	2			5	2

[a] Assumes an initial HO_2NO_2 of 2 ppb at 25 km (from Jesson et al., 1977).

The proposed NO_z instrumentation includes a NO chemiluminescence monitor in series with a high temperature catalytic converter (NO_z channel) along with a second NO chemiluminescence monitor operated in parallel. This instrumentation would permit NO, NO_z, and NO_z-NO measurements. To maintain equivalent flow parameters, e.g. identical residence times, the NO channel would be made equivalent to the NO_z channel except that a uniform low temperature would be employed. Experimental data for an NO_z type channel was presented in paragraphs 3.3.1 and 3.5.2. To better understand the sample reaction kinetics, stratospheric simulations of the sample passing through the instrumentation have been modeled and analyzed by the GEARS/EPISODE code. An understanding of these analyses is required to determine the feasibility of an NO_z or total odd-nitrogen monitor.

Finally, as part of the overall feasibility of NO_z type of instrumentation, wall effects and the propagation of very low levels of certain species are considered by drawing upon vacuum technology in an attempt to develop a physical description of sorption processes. Simulations are treated first, while a baseline design for the sample handling is treated last.

3.9.1 Stratospheric-Based Instrument Modeling

The instrument will naturally induce changes in the incoming ambient air sample. These changes must be minimized if an accurate determination of the unperturbed atmosphere is to be made. These internal changes depend in part on temperature, pressure, specie concentrations, reaction rates and sample flow rate. The calculations have been carried out assuming inviscid flow of a perfect gas at low Reynolds number for several pressures. The instrumentation has been assumed to be athermalized to pre-selected model values and heterogenous reactions have been assumed to be negligible.

The EPISODE code was employed to analyze NO_2, N_2O_5, HNO_3, C ONO_2, and HO_2NO_2 conversions. Criteria for reaction selection was based upon known mechanisms, a reasonable knowledge of the rates, the magnitude of the rate and the reactant number density. Appropriate O_3 reactions were included since $[O_3] \sim 10^{12}$ molecules/cm^3.

The reaction set for N_2O_5 thermal decomposition was listed at the beginning of Paragraph 3.5.1 with the exception of the ozone oxidation of NO to NO_2.

The reaction set for HNO_3 thermal decomposition consists of the Johnston mechanisms listed in Paragraph 3.7.1 for reactions (25) and (26), i.e., HNO_3 in the presence of NO, and the ozone oxidations of NO and NO_2 to NO_2 and NO_3.

Both reaction sets, 16 reactions in total, have been combined and computer printouts of concentration versus time for a 25 km altitude situation are provided in Appendix B. Instrumentation temperatures of 250, 300, 400, 550, 600, 700, and 800 K have been selected. The first two values correspond to instrumentation temperatures where no active thermal heating would be occurring. The last temperature value corresponds to an upper limit value for the conversion of HNO_3 and nearly complete conversion of NO_2.

A portion of the profile data of Appendix B has been selected and the gradient of appropriate species is presented in Table 3-22 for an assumed residence time of 5 seconds and initial concentrations representative of 25 km. These initial concentrations are; NO = 7.0×10^8, NO_2 = 6.2×10^9, N_2O_5 = 7.0×10^8, HNO_3 = 3.0×10^9, O_3 = 4.3×10^{12} and H_2O = 6.0×10^{12} molecules/cm^3. At reduced temperatures, e.g., 250 and 300 K, where one is interested in an $[NO]$ determination, NO is oxidized by O_3 forming NO_2. The loss or measurement bias can be determined with a knowledge of the ambient $[O_3]$, the measurement of $[NO]$, instrumentation temperature and sample flow rate. At the intermediate temperatures tabulated, where conversion of HNO_3 is only partial, the gradient ratio given in the last column shows significant departure from unity. At the higher temperatures tabulated, the ratio converges to unity. The small departure from unity is attributable to a small increase in the $[NO_3]$ and represents a measurement bias error since NO_3 is not measured.

TABLE 3-22. NET CHANGE OF SPECIES (molecules/cm^3) VS TEMPERATURE FOR RESIDENCE TIME OF 5 SECONDS

T(K)	ΔNO	ΔNO_2	$\Delta 2N_2O_5+HNO_3$	$-\Delta NO_2+2N_2O_5+HNO_3 /\Delta NO$
250	-0.090×10^9	$+0.090 \times 10^9$	-0.0	1.000
300	-0.212	+0.219	-0.023×10^9	0.924
400	-0.502	0.119	-1.400	2.551
550	+0.538	+0.042	-1.400	2.524
600	+3.115	-2.487	-1.403	1.249
700	+7.110	-5.554	-1.947	1.054
800	10.18	-6.058	-4.400	1.027

From the data tabulated in this table and various instrumentation parameters cited above, it may concluded that $[NO]$ can certainly be determined and that the summation term $[NO_2 + 2N_2O_5 + HNO_3]$ can be determined at 800 K by differencing the two $[NO]$ measurements after correction for the NO oxidized during instrument transit time. For short duration flights, the use of dry ice is practical for further reducing the oxidation.

A design analysis or tradeoff study employing the EPISODE code to determine altitude, temperature, and residence time effects was conducted to verify the engineering feasibility of a high temperature NO_z converter. Figure 3-18 presents the parametric results of this analysis where the gradient ratio defined in Table 3-22 is plotted against altitude for temperatures of 800 and 900 K and residence times of 1.0, 2.5, and 5.0 seconds.

The sigmoidal shapes of the parameter curves of Figure 3-18 is an artifact of the representative species concentration profiles of the stratosphere selected for the calculation. No analysis was carried out for grossly perturbed profiles.

To minimize the NO_3 measurement bias error, the NO_z high temperature converter should be operated at as high a temperature as practical and retain

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HIGH ALTITUDE POLLUTION PROGRAM STRATOSPHERIC MEASUREMENT SYSTE--ETC(U)
FEB 80 N H MACOY, R WEINGARTEN, A PIRES DOT-FA77WA-4080

UNCLASSIFIED PE-14262 FAA/EE-80-11 NL

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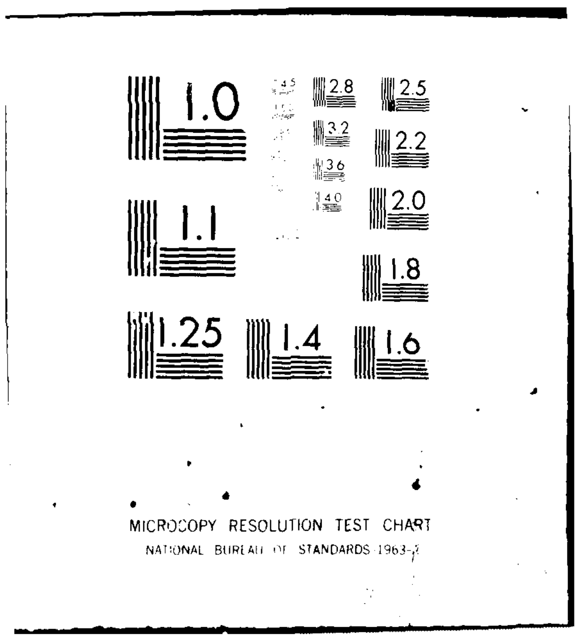
1.0
2.8
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2.2
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MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963

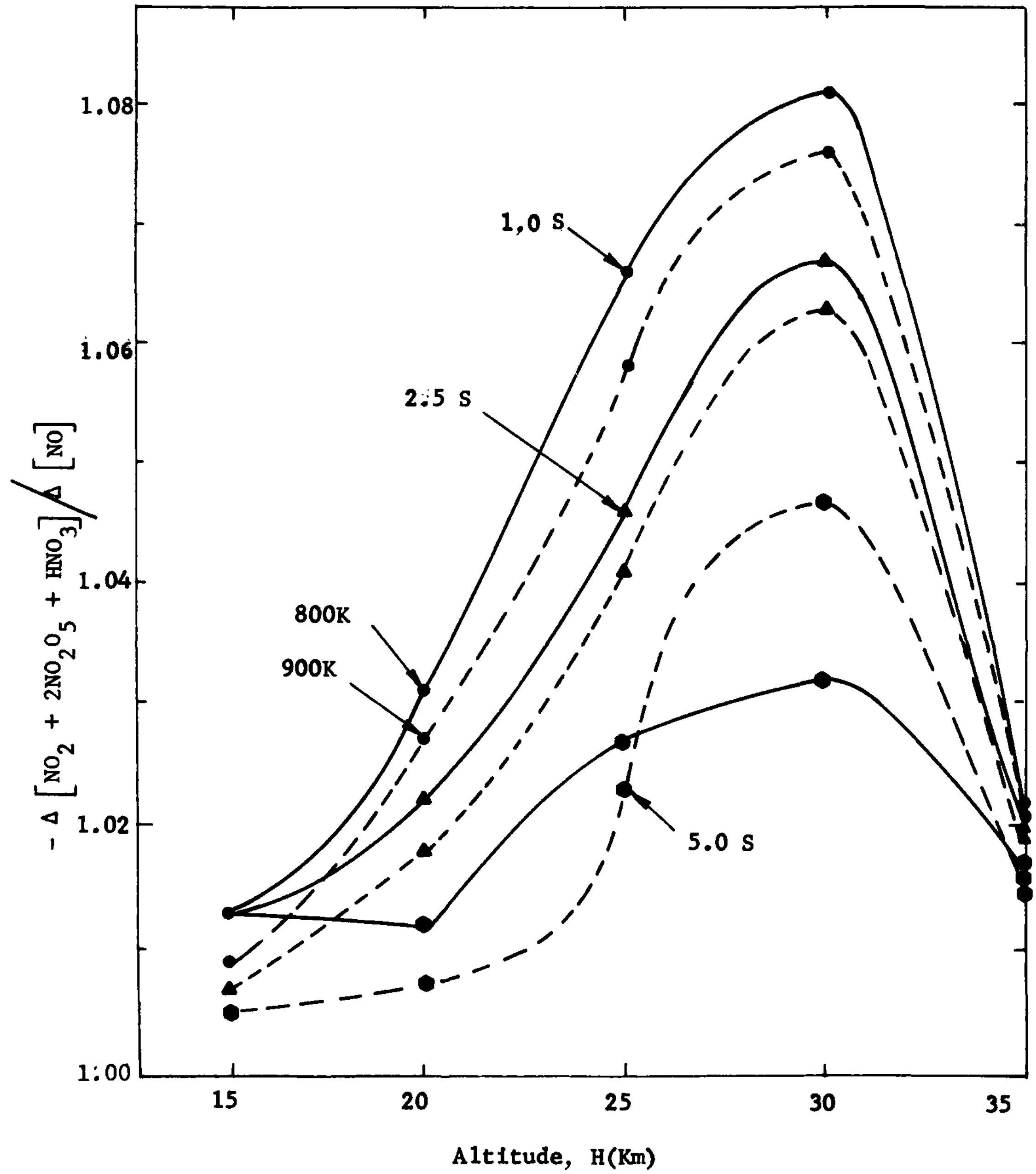


Figure 3-18. NO_3 Measurement Bias Error

the sample for as long as practical. Based upon a temperature of 800 K and a residence time of 5 seconds, Figure 3-18 suggests that the measurement uncertainty will be less than 4 or 5 percent.

The thermally labile species, $ClONO_2$ and HO_2NO_2, were then considered and their decomposition reactions added to the EPISODE code file. The reactions and rates are listed below for reference. The dimensional units are cm^3-molecule^{-1}-s^{-1}.

$$ClONO_2 + M \longrightarrow ClO + NO_2 + M \qquad (-32)$$

$$k_{-32} = k_{-34a} + 1.32 \times 10^{-5} \exp(-11{,}980/T) \left[N_2\right]$$

$$k_{-32a} = 2.74 \times 10^{6} \exp(-3350/T)$$

$$HO_2NO_2 + M \longrightarrow HO_2 + NO_2 + M \qquad (-37b)$$

$$k_{-37b} = 6 \times 10^{17} \exp(-2600/RT)$$

Computer printouts for the expanded set are included in Appendix B for temperatures of 250, 300, 700 and 800 K.

3.9.2 Heterogenous Sample Changes

Internal sample changes will also result if adsorption-desorption phenomena are occurring. Molecular adsorption takes place until a condition of equilibrium with desorption is realized. The following treatment, based on both kinetic theory and activation energy, is adopted from the work of Santeler et al. (1966). For the major species of the stratosphere, H_2O will be of most concern. For water with a molecular weight of 18, the surface concentration (ideal monolayer) S_m is, from kinetic theory,

$$S_m(300\text{ K}, 18) = 3.7 \times 10^{-5}\text{ torr-liter/cm}^2 = 1.2 \times 10^{13}\text{ molecules/cm}^2$$

$$S_m(800\text{ K}, 18) = 6.0 \times 10^{-5}\text{ torr-liter/cm}^2 = 2.0 \times 10^{13}\text{ molecules/cm}^2$$

for temperatures of 300 and 800 K, respectively. At a pressure of 0.1 atm, the time needed to form a monolayer is about 33 nS.

Applying the activation energy concept for residence time gives

$$t_r = t_o \exp (\Delta E/RT)$$

where t_o = the vibrational period of the lattice, 10^{-13}s at 300 K

E = characteristic energy, 24,000 cal/gm-mole

R = gas constant, 1.986 cal/deg-mole

T = temperature, 300 or 800 K

Therefore, $t_r = 3 \times 10^4$ and 3.6×10^{-7} seconds for the low and high temperatures. Thus one can expect that the room temperature NO instrumentation ahead of the gas phase titration region will scavenge N_2O_5 and possibly HNO_3 from the sample stream. Conversely, the 800 K NO_z instrumentation ahead of the gas phase titration region will not scavenge either N_2O_5 or HNO_3 from the sample stream. A recommended preflight task, however, is a thermal vacuum cycling of the high temperature converter.

Finally, it is recommended that all materials exposed to the sample during handling be restricted to glass; quartz; corrosion resistant steels, such as hastelloy, monel, inconel, nickel, gold, or Durimet 20™; or the austenitic steels, such as stainless steel 316 (Grade CF8M) for general use or stainless steel 347 (Grade CF8C) should welding be required; and finally polytetrafluorethylene (PTFE). Glasses and metals should be scrupulously cleaned in benzol and distilled acetone while the polymer materials should be used in the as-processed condition. The use of polymer materials is a controversial subject. In studying part per trillion levels of NO, NOAA scientists have found that, at that level, NO may or may not interact with PTFE, depending upon the ambient humidity (MacFarland, private communication, 1979). Reactivity is reduced to acceptable levels when humidity is low.

3.9.3 NO_z Baseline Design

This section considers the sample handling design for an NO_z converter and NO monitor. A discussion of payload consumables, signal processing, and many other engineering details are therefore missing.

The basic design includes three reaction volumes, sample ingress and egress ports, and reaction volume interconnections. The three reactions volumes are defined to be: (1) the high temperature NO_z converter, (2) an instrument zeroing or background volume where O_3 is injected periodically to consume ambient NO, so as to establish a zero level signal, and (3) a chemiluminescence volume where gas phase titration of O_3 and NO occur. From the data of Figure 3-18, a baseline flow rate of 1 SLPS is selected. This rate would be derived from a servo controlled motor operating a high efficiency-zero-head lobe pump such as employed by NOAA (Drummond, private communication, 1979). This method of sample transport has two immediate advantages: (1) the flow rate is independent of ambient pressure and (2) once the pump and motor are characterized, an on-board flow meter is not required.

A general description follows. Upon sample entry to the instrumentation, the sample is exposed to a high temperature catalytic furnace or reaction vessel where NO_z is converted to NO. For monitoring of only NO, the sample passes through a similar and parallel vessel whose temperature is maintained below 300 K. Each channel contains a pre-reaction vessel where O_3 may be periodically injected to generate a zero-reference level. Provision for injecting known levels of NO and NO_2 are also included for calibration purposes.

The design layout for the NO_z converter/NO monitor is shown in Figure 3-19. The NO monitor reaction vessel design closely approximates the design used by NOAA for tropospheric sensing of NO. The design has been altered for stratospheric sensing.

The NO_z moderate temperature reaction vessel is spherically shaped to maximize the volume to surface ratio. The volume, 4070 cm^3, was selected to provide a residence time of about 5 seconds, actually 4 seconds at a flow rate of 1 SLPS. A platinum-rhodium heating filament on an alumina support and sample ingress-egress deflection baffles of stainless steel material will be located within the sphere. The platinum filament serves two functions. First, as catalyst, it promotes the conversion of NO_2 to NO as discussed in paragraph 3.3.1. Secondly, it tends to scavenge atomic oxygen by surface

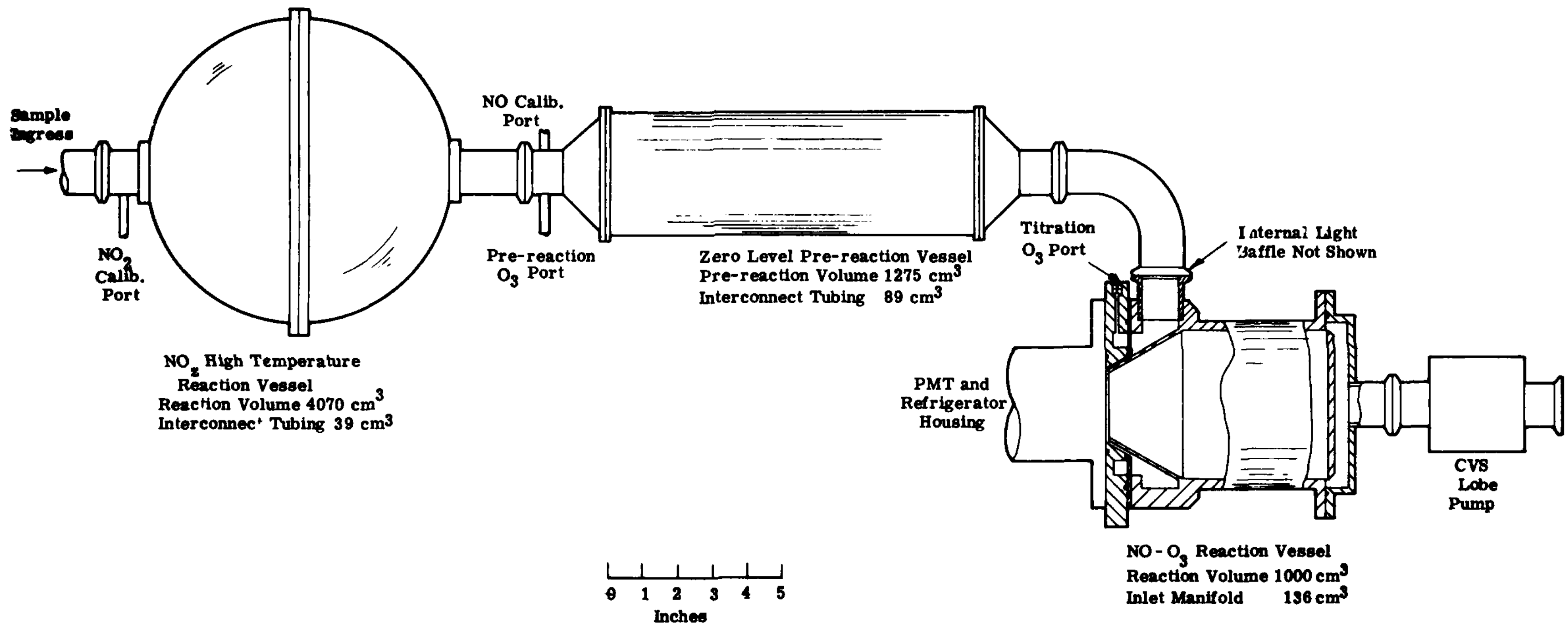


Figure 3-19. NO_z Converter - NO Sensor Flow Layout

recombination produced by the thermal decomposition of O_3. To minimize conductive heat losses, the sample ingress and egress flanges and tubing would be constructed of gold plated, thin walled, commercially pure titanium since titanium has a low heat conductivity.

The design details for the high temperature NO_2 catalytic converter used in the laboratory as well as the moderate temperature NO_z catalytic converter are given in Table 3-23.

The function of the zero level pre-reaction vessel permits chemiluminescence to occur before the sample reaches the photomultiplier tube, thereby allowing the PMT counter to accumulate a base level dark count. This count is then used as the zero reference level. The ozone is injected 1500 cm^3 ahead of the titration ozone manifold. At a sample flow rate of 0.25 SLPS, the residence time is 6 seconds. Using expressions 3-6 and 3-7, and the O_3 parameters of paragraph 3.1.1, yields

$$\frac{\Delta[NO]}{[NO]} = 1 - \exp(-4.9) = 0.983$$

at an altitude of 25 km so that all but 0.7 percent of the NO is consumed ahead of the $NO\text{-}O_3$ reaction vessel. At reduced altitudes the reaction is more complete.

The $NO\text{-}O_3$ reaction vessel contains an ozone inlet manifold and a sample inlet manifold. Mixing is initiated concentrically about the axis of the vessel near the PMT end of the vessel. At the opposite end of the vessel, a gold coated mirror is placed in conjunction with the gold plated cylindrical vessel to form a photon integrating cavity. A sample pumping port and lobe motor pump are located behind the mirror. For a sample residence time of 4 seconds, the data of Table 3-1 predicts total conversion to NO_2 of which about 7.2 percent is converted to the optically active state $^2B_1$.

3.10 POTENTIAL OF A NEW TECHNIQUE FOR NO_2 MEASUREMENTS

J.G. Anderson of Harvard University (private communication, 1979) is making laboratory measurements on a new technique for the measurement of NO_2.

TABLE 3-23. HIGH TEMPERATURE REACTION VESSEL DESIGN COMPARISON

Parameter	Aerochem NO_2 Converter	Perkin-Elmer Converter	Relative Factor
Flow Rate	0.035 SLPS	1.0 SLPS	28.6
Temperature	~ 1373 K	~ 800-900 K	-
Ambient pressure	1000 mb	6 to 120 mb	-
Filament material	Pt 10% Rh	Pt 10% Rh	-
Filament casing	McDanel Refractory 99% alumina	Omega Engineering 99% alumina	-
Bonding material	Aremco Ultrabond 552	Sodium Silicate cement or Ultra-bond 552	-
Filament size	Avg No.30 (0.010")	Avg No. 24 (0.020")	-
Filament length	120 inches	600 inches	5.0
Contiguous sample volume	1.14 cm^3	26 cm^3	22.7
Contiguous sample residence time	33 mS	26 mS	0.8
Contiguous filament surface area	27.9 cm^2	235 cm^2	8.4
Heat equivalent power	14 watts	11 watts @ 50 mb	-

This new technique is very similar to the technique recently used for water vapor measurements in the stratosphere (Kley and Stone, 1978) and was suggested in the same report. The technique consists of the photodissociation of NO_2 using Lyman alpha (1216 A) light and the detection of the characteristic gamma-band fluorescence of the excited NO produced.

$$NO_2 + h\nu\ (1216\ A) = NO(A^2\ \Sigma^+) + 0 \qquad (3\text{-}45)$$

$$NO(A^2\ \Sigma^+) = NO + h\nu\ (1900\ A) \qquad (3\text{-}46)$$

The detected signal in cts/sec-molecule/cc is proportional to the fluorecence intensity multiplied by optical efficiencies and by geometrical factors. The fluorescence intensity can be expressed by

$$I = \frac{\left[NO_2\right] \cdot J \cdot \emptyset \cdot A}{A + \ air\ \ K_q^{air}} \qquad (3\text{-}47)$$

The photodissociation process is described by $\emptyset$, the quantum yield, and by J, the photodissociation coefficient. This coefficient is related to the light source photon flux ψ and the absorption cross section, σ_λ ,

$$J = \psi_\lambda \sigma_\lambda \qquad (3\text{-}48)$$

The fluorescence process is described by A, the transition probability per second, and k_q^{air}, the quenching rate coefficient for air.

.reliminary results of Anderson indicate that the sensitivity of the technique is 5×10^{-8} cts/sec-molecule/cc or about 10^8 molecules/cc of NO_2 at a S/N of 1. His results indicate a quantum yield smaller than 1% for all gamma-bands. This photoyield is smaller than that of H_2O for $OH(A^2\ \Sigma^+)$ and smaller than anticipated (Kley and Stone, 1978). Anderson is considering means to improve the sensitivity, and Kley (private communication, 1979) will also make laboratory measurements. These means are, to select a better photolyzation wavelength where either the cross section or quantum yield is larger or to utilize a more intense source according to 3-47 and 3-48. The present sensitivity is adequate to meet the HAPP requirements.

Several specificity issues remain to be studied, but are not expected to affect the NO_2 measurements. The photolyzing radiation will act on all stratospheric species and could produce interfering fluorescence or secondary fluorescence. The low quantum yields mean that secondary fluorescence (i.e., NO_2 fluorescence from an NO_2 product of another dissociation) will be very

small. One does not expect interfering fluorescence from other product species. On the contrary, these product species may themselves be measured at the same time using other spectral channels. Complete identifications of their parents may, however, require use of several excitation wavelengths (Kley and Stone, 1978). Finally, the need to view as much fluorescence from excited NO as possible could cause acceptance of scattered sunlight.

The demonstration of this dissociation/fluorescence technique for NO_2 would also lead to a more specific technique for NO. One would convert the NO to NO_2 using titration with O_3 as is done in the chemiluminescence technique for NO. Its drawback is that NO_2 concentrations are usually larger than NO and so one would lack sensitivity for NO concentrations much lower than NO_2 concentrations (e.g., during sunrise, sunset, and night).

The new technique for NO_2 promises both sensitive and specific measurements of NO_2 in a lighter and more compact module than the broadband dissociation module. If all these potentials are demonstrated, the dissociation/fluorescence technique should replace the broadband technique in the Hybrid Gas Conversion System. Flight demonstration may be carried out in 1979 by Anderson in his configuration of a fast-flow, parachute drop payload. This configuration is not essential to the technique, which is also applicable to the slow-flow sampling envisioned for the HAPP Stratospheric Measurement System. Slow-flow sampling and calibration techniques have been demonstrated for NO in the stratosphere (B.A. Ridley, et al., 1972).

SECTION IV

CONCLUSIONS AND RECOMMENDATIONS

This section is devoted to conclusions drawn from the experimental work as well as the analytical work undertaken during this program. A summary of this work is given in Section II.

Recommendations are also presented in the context that only hybrid chemical conversion techniques were reported upon. The validity of the hybrid technique for carrying out the scientific and engineering objectives of the HAPP Stratospheric Measurement System is paramount. The merits of only this system are considered in developing a recommended position. Where appropriate, further areas of investigation, again only for this type of system, are recommended.

4.1 CONCLUSIONS

Conclusions for the laboratory findings associated with molecular chemical conversion techniques are arranged in the same order as the evaluation of the technique appeared in Section III.

Measurement of stratospheric NO is basically carried out by gas phase titration with O_3 immediately followed by the sensing of the chemiluminescence of the product molecule, NO_2^*. With laboratory instrumentation used in this study, a sensitivity of 1.6×10^{10} molecules/cm^3 could be routinely measured. With stratospheric instrumentation, a lowest detection limit of 5×10^7 molecules/cm^3 has been verified (B.A. Ridley, et al., 1972).

Conversion of NO_2 to NO and $O(^3P)$ by the photolytic process is complex and may result in substantial changes of the relative concentrations of other species in the sample stream. These changes in turn can bias the readings. In addition, dissipated heat from the photolytic lamp could assist in the

premature thermal decomposition of N_2O_5, and certainly $ClONO_2$ and HO_2NO_2, the latter two species being particularly labile and believed to be present in the stratosphere. Further, as shown in the Feasibility Study Report, this method requires substantial amounts of electrical power derived from light weight primary cells or heavier secondary cells. Reduction of the premature decomposition of N_2O_5, $ClONO_2$ and HO_2NO_2 to negligible levels would require that the photolytic cell be packed in dry ice. A lowest detection limit of about 1×10^8 molecules/cm^3 is achievable but depends upon engineering trades relating electrical power and radiated flux.

Concerning the measurement of N_2O_5 the conclusions may be grouped into categories of (1) generation and handling of N_2O_5 in known quantities and (2) conversion of N_2O_5 into product molecules which can be quantitatively measured. Firstly, ppm quantities of N_2O_5 can be easily generated, the process followed by IR absorption techniques followed in turn by stoichiometric and rate limiting evaluations. Handling of N_2O_5 is more difficult because water tends to combine, thus forming HNO_3. This artifact of the generation and handling of N_2O_5 can be routinely evaluated by monitoring the IR signature of HNO_3. Secondly, thermal conversion of N_2O_5 is complete at temperatures in the 450-473 K range. Obtaining a measurable decomposition product quantitatively, however, is not straightforward. For example, computer analysis shows that at an altitude of 15 km, the net change of NO_3 exceeds the net change of N_2O_5; while at a altitude of 25 km, the net change of NO_3 is less than the net change of N_2O_5. Computer analysis and laboratory tests at higher temperatures, up to and including 800 K, indicate that the thermal conversion process becomes substantially more quantitative. At this point on the temperature scale, however, specificity to HNO_3 is lost, leading to the concept of NO_z instrumentation.

Thermal conversion of HNO_3 is a non-catalytic process, but one that requires a surface. Surface materials employed during this program included Pyrex and stainless steel. Temperature ranges employed were 520-550 K for Pyrex and up to 673 K for stainless steel. Thermal decomposition of HNO_3 was found to be complete at the lower temperature range with the principal

product being NO_2. A quantitative portion of the NO_2 is thermally converted to NO. Stoichiometry of the conversion to NO_2 prior to allowance for NO_2 thermal decomposition was found to be unity within experimental error. In summary, the conversion of HNO_3 to NO_2 and NO was found to be straightforward for concentrations as high as 1.7×10^{14} molecules/cm^3.

Interferents impacting the specificity of thermal conversion instrumentation include $ClONO_2$ and HO_2NO_2 to the extent that they are present in the stratosphere. Conversion of HO_2NO_2 will be present for temperatures ≥ 300 K. Conversion of $ClONO_2$ will be present for temperatures ≥ 350 K.

Conversion of total odd-nitrogen, to measurable NO, without regard to specificity, can be carried out using the high temperature catalytic thermal technique. The stoichiometry of the various molecules, HNO_3, N_2O_5, $ClONO_2$, HO_2NO_2 and NO_2 is well understood. Passage of the sample through a converter operated at 500-800 K would decompose the heavier molecules, including NO_2, at stratospheric pressures. The resulting product, NO, would then be measured by the GPT-chemiluminescence method. Measurement of only NO would be carried out in an identical, parallel path but without thermal conversion.

The narrow-band photolysis/fluorescence technique for NO_2 is being investigated by J. Anderson in the laboratory. His best result thus far indicates a sensitivity of about 10^8 molecules/cc, which meets the HAPP NO_2 specification. Specificity is not expected to be a problem. Conversion of NO to NO_2 by titration with ozone may allow the same technique to measure NO to the same precision. Anderson tentatively plans a demonstration flight during 1979 in his unique parachute package. The same technique is applicable to the slow-flow sampling envisioned for the HAPP Stratospheric Measurement System. In both cases, on-board calibration is advisable.

The GEARS/EPISODE computer code was found to be a valuable analytic modeling tool for developing laboratory apparatus as well as for developing design and performance parameters for instrumentation intended for stratospheric conditions. The modeling results for both laboratory conditions and those

for expected concentrations of the stratosphere indicate, with only minor differences, identical conversion trending. This permits valid extrapolation of the laboratory results. The code provides a rigorous analysis that will also benefit pre-launch and in-flight calibration tasks.

Sample fidelity, transport, radical chemistry and surface reactions which are not amenable to modeling must be given particular attention in the instrumentation design, use and interpretation of data.

4.2 RECOMMENDATIONS

From the results of the Feasibility Study and the results of the laboratory performance studies reported here, Perkin-Elmer recommends the development of a flight prototype of the Hybrid Gas Conversion Measurement System. It is recommended that the flight prototype consist of a number of instrumentation modules that can be improved, changed, or added to achieve the scientific objectives of the High Altitude Pollution Program. Candidate modules are the total odd-nitrogen (including NO) module, the NO_2/NO module, the O_3 module, and the N_2O module. Measurements with these modules would meet all requirements on the Stratospheric Measurement System except the partitioning of the heavier odd-nitrogen species. Each of these modules is considered to be feasible from an engineering point of view. It may be possible to add a partitioning module at a later time, depending on the technology of stratospheric measurements. In no case, however, would a module be flown before testing in the laboratory under stratospheric conditions.

Perkin-Elmer recommends that the development of a flight prototype of the Total Odd-Nitrogen Instrumentation Module be initiated. Functional design would be based upon chemiluminescence detection for NO and high-temperature catalytic conversion for the HNO_3, N_2O_5, NO_2, and other odd-nitrogen species. As documented in this report, the measurement technique is demonstrated under laboratory conditions, no new technology is being advanced, and none of the module components are state-of-the-art. This development should be carried out jointly by the system contractor and a stratospheric chemistry laboratory group.

Perkin-Elmer further recommends that the development of a flight prototype NO_2/NO Instrumentation Module be initiated. This module is essential for obtaining the important measurements of NO_2. Functional design would be based upon chemiluminescence detection of NO and the narrowband photolysis fluorescence technique for NO_2 if that technique is demonstrated in the stratosphere as expected. In this case, a balloon version of the latter technique would have to be developed. If the narrow-band photolysis techniques does not work as expected, the broad-band photolysis technique should be further optimized for NO_2 detection as indicated in this report.

Perkin-Elmer also recommends that two other Instrument Modules be considered as part of the flight prototype at this time. These modules are the flyable gas chromatograph for N_2O and the UV photometer for O_3. Both modules are in states of advanced development and testing. The flyable gas chromatograph is being developed by Valco Instruments and Baseline Instruments and is being tested by NOAA in Boulder. The flyable UV photometer is made by DASIBI Environmental Corporation and has been tested by NASA Johnson Space Center.

Perkin-Elmer finally recommends that provision be included in a flight prototype for one or two other instrumentation modules. The volume set aside could be utilized for batteries, permitting longer flights until additional candidate modules are developed.

REFERENCES

Aerochem Research Laboratories, Inc., Instruction Manual for Chemiluminescence Monitor, Model AA-35, Aerochem TP-286f, 1977.

Altshuller, A.P., "Thermodynamic Functions for Nitrogen Dioxide and Nitrous Acid", J. Phys. Chem., 61, 251, 1957.

Anderson, Larry G., "Atmospheric Chemical Kinetics Data Survey," Revs. Geophys. & Space Physics, 14, 151, 1976.

Atkinson, R., et al. "Rate Constants for the Reactions of the OH Radical with NO_2 (M = Ar and N_2) and (M = Ar)", J. Chem. Phys., 65. 306, 1976.

Birks, John W. et al., "Studies of Reactions of Importance in the Stratosphere II. Reactions Involving Chlorine Nitrate and Chlorine Dioxide", J. Chem. Phys. 66, 4591 (1977).

Breitenbach, L.P. and M. Shelef, "Development of a Method for the Analysis of NO_2 and NH_3 by NO-Measuring Instruments," JAPCA 23, 128, 1973.

Clyne, M., et al., "Kinetics of the Chemiluminescent Reaction between Nitric Oxide and Ozone," Trans. Faraday Soc., 60, 369, 1964.

Clough, P.N., and B.A. Thrush, "Mechanism of Chemiluminescent Reaction between Nitric Oxide and Ozone," Trans. Faraday Soc., 63, 915, 1967.

Constant, Jr., Paul C., Michael C. Sharp and George W. Scheil, "Collaborative Test of the Chemiluminescent Method for Measurement of NO_2 in Ambient Air," Midwest Research Institute, Kansas City, MO., EPA Rpt 650/4-75-013, 1975. See also Rehme, K.A., B.E. Martin and J.A. Hodgeson, "Tentative Method for the Calibration of Nitric Oxide, Nitrogen Dioxide and Ozone Analyzers by Gas Phase Titration," U.S. Environmental Protection Agency RTP, EPA-R2-73-246, 1974.

Cox, R.A., R.G. Derwent and A.E.J. Eggleton, Chlorine Nitrate - A Possible Stratospheric Sink for ClO Radicals and NO_x with Significant Implication for Ozone Depletion, U.K. Atomic Energy Authority-Harwell, AERE-R 8383, 1976.

Federal Register 38, #136, 19094, 1973.

Fontijn, A., et al., "Homogeneous Chemiluminescent Measurement of Nitric Oxide with Ozone," Anal. Chem., 42, 575, 1970.

Frejacques, Claude, "The Kinetics of Decomposition of Nitric Acid in the Vapor Phase," Compt. Rendus, 232, 2206, 1951.

Gear, C. William, Numerical Initial Value Problems in Ordinary Differential Equations, Prentice-Hall Inc., Englewood Cliffs, NJ, 1971.

Gelbwachs, J.A., et al., "Fluorescence Determination of Atmospheric NO_2," Opto-Electronics, 4, 155, 1972.

Goldman, A., et al., "Statistical Band Model Parameters and Integrated Intensities for the 5.9 m, 7.5 m and 11.3 m Bands of HNO_3 Vapor," Appl. Opts., 10, 65, 1971.

Goldman, A., F.S. Bonomo, W.J. Williams, and G.G. Murcray, "Absolute Integrated J. Quant. Spectrosc. Radiat. Transfer, 15, 107, 1975.

Graham, R.A., Ph. D. Thesis, University of California, Berkley, 1975. See also Graham, Richard A., and Harold S. Johnston, "The Photochemistry of NO_3 and the Kinetics of the N_2O_5-O_3System," J. Phys. Chem. 82, 254, 1978.

Graham, R.A., E.C. Tuazon, A.M. Winer and J.N. Pitts, Jr., "High Resolution Infrared Absorptivities for Gaseous Chlorine Nitrate" Geo. Res. Ltrs. 4, 3, 1977.

Graham, Richard A., Arthur M. Winer and James N. Pitts Jr., "Temperature Dependence of the Unimolecular Decomposition of Pernitric Acid and its Atmospheric Implications," Chm, Phys. Ltrs. 51, 215, 1977.

Graham, Richard A., Arthur M. Winer and James N. Pitts Jr., "Pressure and Temperature Dependence of the Unimolecular Decomposition of HO_2NO_2," J. Chem. Phys. 68, 4505, 1978.

Hampson, Jr., Robert F. and David Garvin, Chemical Kinetics Data Survey VI, U.S. Dept. of Commerce, NBS Internal Report 73-207, 1973.

Hampson, Jr., Robert F. and David Garvin, Reaction Rate and Photochemical Data for Atmospheric Chemistry - 1977, U.S. Dept. of Commerce, NBS Special Publication 513, 1978.

Howard, Carleton J., and K.M. Evanson, "Kinetics of the Reaction of HO_2 with NO," Geophys. Res. Lett., 4, 437, 1977.

Hindmarsh, A.C., and Byrne, G.D. EPISODE: An Experimental Package for the Integration of Systems of Ordinary Differential Equations, Lawrence Livermore Laboratory Report UCID-30112 (1975).

Jesson, J.P., et al., "The Stratospheric Abundance of Peroxynitric Acid," Geophys. Res. Lett., 4, 513, 1977.

Johnston, Harold S., "Four Mechanisms Involving Nitrogen Pentoxide," J. Amer. Chem. Soc. 73, 4542, 1951.

Johnston, H.S., et al., "The Kinetics of the Thermal Decomposition of Nitric Acid Vapor," J. Amer. Chem. Soc., 73, 2319, 1951.

Johnston, H.S., et al., "The Kinetics of the Thermal Decomposition of Nitric Acid Vapor. II: Mechanism," J. Phys. Chem., 57, 390, 1953.

Johnston, H.S. et al., "The Kinetics of the Thermal Decomposition of Nitric Acid Vapor. III: Low Pressure Results," J. Amer. Chem. Soc., 77, 4208, 1955.

Johnston, H.S., and H.J. Crosby, "Kinetics of the Fast Gas Phase Reaction between Ozone and Nitric Oxide," J. Chem. Phys., 22, 689, 1954.

Johnston, H.S., and R. Graham, "Photochemistry of NO_x and HNO_x Compounds," Can. J. Chem., 52, 1415, 1974.

Kley, D., and E.J. Stone, "Measurement of Water Vapor in the Stratosphere by Photodissociation with Ly α (1216 A) Light," Rev. Sci. Inst. 49, 691 (1978).

Knauth, H.D. "Uber den thermischen Zerfall von $ClONO_2$ in Gegenwart von NO, ClNO and N_2," Ber. Bunsenges. Phys. Chem. 82, 212, 1978.

Luther, F.M., Lawrence Livermore Laboratory First Annual Report to the High Altitude Pollution Program, Report No. FAA-EQ-77-6, 1976.

Macoy, Norman H., Sherman K. Poultney, Lloyd M. Logan and Mary Rotheram, High Altitude Pollution Program Stratospheric Measurement System Feasibility Study, Report No. FAA-AEQ-78-10, 1978.

Miller, David F., et al., "A Versati. Electrochemical Monitor for Air Quality Measurements," J. Air Poll. Control Assoc., 21, 414, 1971.

Miller, R.H., D.L. Bernitt and I.C. Hisatsume, "Infrared Spectra of Isotopic Halogen Nitrates," Spectrochimica Acta, 23A, 223, 1967.

NASA (National Aeronautics and Space Administration), Chlorofluoromethanes and the Stratosphere, Report RP-1010, September 1977.

Nightingale, R.E., et al., "Preparation and Spectra of Nitrogen Oxides," J. Phys. Chem., 58, 1047, 1954.

Niki, H., et al., "Fourier Transform IR Spectroscopic Observation of Pernitric Acid Formed via HOO + $NO_2 \longrightarrow HOONO_2$," Chem. Phys. Lett., 45, 564, 1977.

Pitts, Jr., James N., John M. McAfee, William D. Long and Arthur M. Winer, "Long-Path Infrared Spectroscopic Investigation at Ambient Concentration of the 2% Neutral Buffered Potassium Iodide Method for Determination of Ozone," Env. Sci. Tech. 10, 787, 1976.

Ridley, B.A., et al., "Instrumentation for NO Measurement in the Stratosphere," Proc. Second Conf. on CIAP, Rpt. No. DOT-TSC-OST-73-4, U.S. Department of Transportation, 146, 1972.

Ridley, B.A., et al., "Measurement of Nitric Oxide in the Stratosphere Between 17.4 and 22.9 km," Planet. Space Sci., 22, 19, 1974.

Ridley, B.A., and H.I. Schiff, In-Situ NO_x Measurements Progress Report, York University, Contr DOT-FA77WA-3931, Feb. 1978.

Schack, Carl J., "A New Synthesis of Chlorine Nitrate," Inorganic Chem. 6, 1938, 1967.

Schmeisser, M., Handbook of Preparative Inorganic Chemistry Vol. I, 2nd edition, Ed. by Georg Braner, Academic Press, N.Y., p326, 1963.

Schott, Gary and Norman Davidson, "Shock Waves in Chemical Kinetics. The Decomposition of N_2O_5 ac HIgh Temperatures," J. Amer. Chem. Soc., 80, 1841, 1958.

Simonaitis, R., and Julian Heicklen, "Reaction of HO_2 with No and NO_2," J. Phys. Chem., 78, 653, 1974.

Simonaitis, R., and Julian Heicklen, The Temperature Dependence of the Reactions of HO_2 with NO and NO_2, Ionsphere Research Laboratory, Pennsylvania State University, Scientific Report 454, 1977.

Stedman, D.H., and H. Niki, "Kinetics and Mechanism for the Photolysis of Nitrogen Dioxide in Air," J. Phys. Chem., 77, 2604, 1973.

Wilson, G.L., and F.D. Miles, "The Partial Pressures on Nitric Acid - Water Mixtures from 0 - 20 C," Trans. Faraday Soc., 36, 356, 1940.

Wu, C.H., E.D. Morris, Jr., and H. Niki, "The Reaction of Nitrogen Dioxide with Ozone," J. Phys. Chem. 77, 2507, 1973.

APPENDIX A

INFRARED ABSORPTION MEASUREMENTS

A.1 N_2O_5 AND HNO_3 CONCENTRATION DETERMINATION

Prior to evaluating a particular analytical method for a species, as well as following the course of a reaction, IR band spectra were recorded to obtain the quantitative concentration of the species.

The analytical method (Lambert-Beer's Law) was employed using band model absorption cross sections. The method utilized either a Perkin-Elmer Model 521 or Model 580 spectrophotometer equipped with an ambient temperature Foxboro/Wilks 20-meter cell lined with PTFE. Because of the corrosive nature of HNO_3, the KBr windows usually used were replaced with AgCl windows. In all cases, the sample and diluent carrier were allowed to flow freely through the cell. Measurements were carried out at ambient pressure, 747-755 torr and temperature, 296-298 K.

The number density, N, or partial pressure p of the species was calculated on the basis of the Lambert-Beer Law:

$$N = \frac{\ln\left(\frac{I_o}{\sigma I}\right)}{\sigma L} \quad \text{(molecules/cm}^3\text{) and}$$

$$p = \frac{RT \ln\left(\frac{I_o}{I}\right)}{N_{Av} L} \quad \text{(torr)}$$

where: $\ln\left(\frac{I_o}{I}\right)$ corresponds to the base e absorbance

σ = effective cross section in cm^2/molecule

L = pathlength in cm

R = gas constant = 62366 torr-cm^3/mole-K

T = temperature of the sample during measurement

N_{Av} = Avogardro's number = 6.023×10^{23} molecules/mole

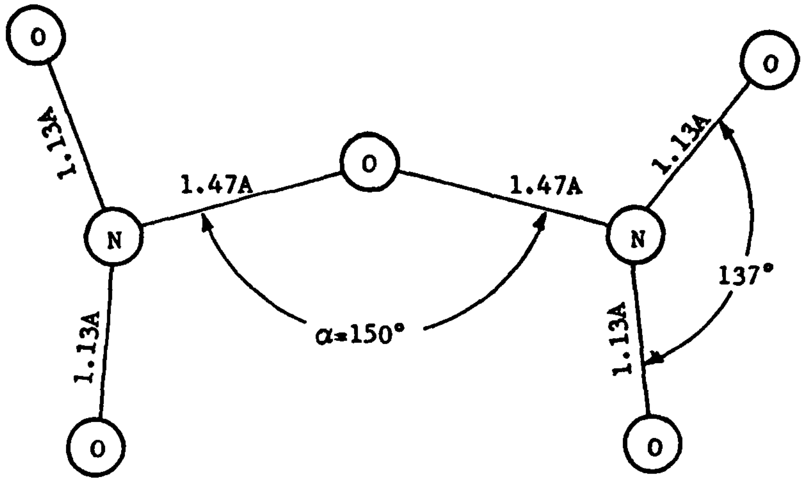
N_2O_5 and HNO_3 have similar molecular structures, as shown in Figure A-1 (Hisatune et al., 1962 and McGraw et al., 1965). Therefore, low resolution spectra may occur at the same frequencies. The ν_1 asymmetric N-O stretch, A_1 symmetry, and ν_{11} asymmetric N-O stretch, B_2 symmetry, modes of N_2O_5 are shown schematically. These modes are observed at a frequency of about 1728 cm^{-1}. The ν_2 asymmetric N-O stretch mode (R-branch) of HNO_3 is observed at about 1720 cm^{-1}.

If both species are present, then the ν_2 band for HNO_3 cannot be used for quantitative measurements without other spectral information*. In cases where two materials are present in a sample mixture, each absorbing at the same frequency or frequencies, the mixture can be analyzed for the concentration of each component by determining the absorbance for the mixture at two or more frequencies.

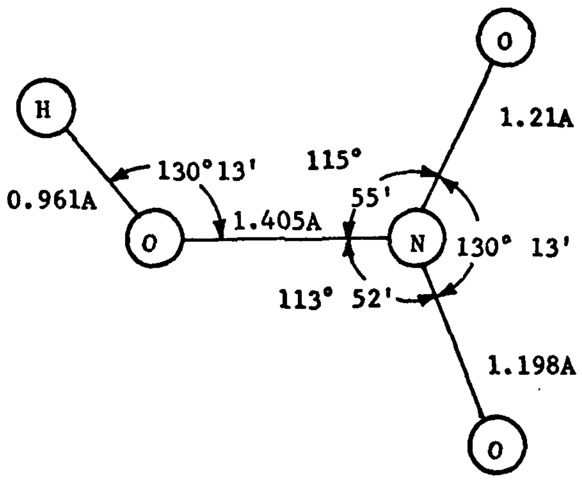
$$A_{e,\nu} = \sigma_{A,\nu} N_A L + \sigma_{B,\nu} N_B L$$

where $A_{e,\nu}$ denotes absorbance to the base e at frequency ν and the subscripts A,B denote N_2O_5 and HNO_3. The cross section, σ, as obtained from the data of Nightingale et al., (1954); Goldman et al., (1971); Goldman et al., (1975); and Graham (1975) are tabulated in Table A-1.

* With the synthesis and handling of N_2O_5 the possibility exists for heterogeneous wall reactions if adsorbed water is present. The product of the reaction is HNO_3 since H_2O_5 is the anhydride of HNO_3.



$O_2N\text{-}O\text{-}NO_2$



$H\text{-}O\text{-}NO_2$

Figure A-1. Molecular Structures for Nitrous Pentoxide and Nitric Acid

TABLE A-1. INFRARED ABSORPTION BAND CROSS SECTIONS FOR N_2O_5 AND HNO_3 (cm^2/molecule)

	Frequency (cm^{-1})			
	1728	1340	1315	1246
A = N_2O_5	2.4×10^{-18}	0.15×10^{18}	0.02×10^{18}	1.75×10^{-18}
B = HNO_3	0.82	0.76	0.98	0.00

From the general expression for absorbance and the data of Table A-1, one may derive the working expressions for number densities as:

$$N_A = \frac{A_{1728} - 1.08A_{1340}}{2.28 \times 10^{-18}L} = \frac{1.19A_{1728} - A_{1315}}{2.85 \times 10^{-18}L} = \frac{A_{1246}}{1.75 \times 10^{-18}L}$$

$$N_B = \frac{A_{1728} - 1.37A_{1246}}{0.82 \times 10^{-18}L} = \frac{A_{1340} - 0.086A_{1246}}{0.76 \times 10^{-18}L} = \frac{A_{1315} - 0.011A_{1246}}{0.98 \times 10^{-18}L}$$

A.2 BAND MODEL CROSS SECTIONS

For reference purposes the band model cross sections for the various gases considered during the program are listed. This data was utilized when low resolution IR spectroscopy was employed as a laboratory analytical method for monitoring reactions and concentrations. The spectral resolution of the instrument is also provided. In all cases the data presented corresponds to room temperature data. Where possible, the most accepted data is employed. A summary chart of the medium strength and stronger bands is presented in Figure A-2.

A.2.1 Nitric Oxide

The data presented for the ν_1 band was taken from laboratory measurements utilizing a Perkin-Elmer model 580 spectrometer set at resolutions of 2.8 and 1.0 cm^{-1}. The 1.0 cm^{-1} data corresponds to the envelope of the resolved lines of the P and R branches. The NO gas at 6 torr was pressure broadened by N_2 with a total pressure of 760 torr. A path length of 8.25 meters was employed.

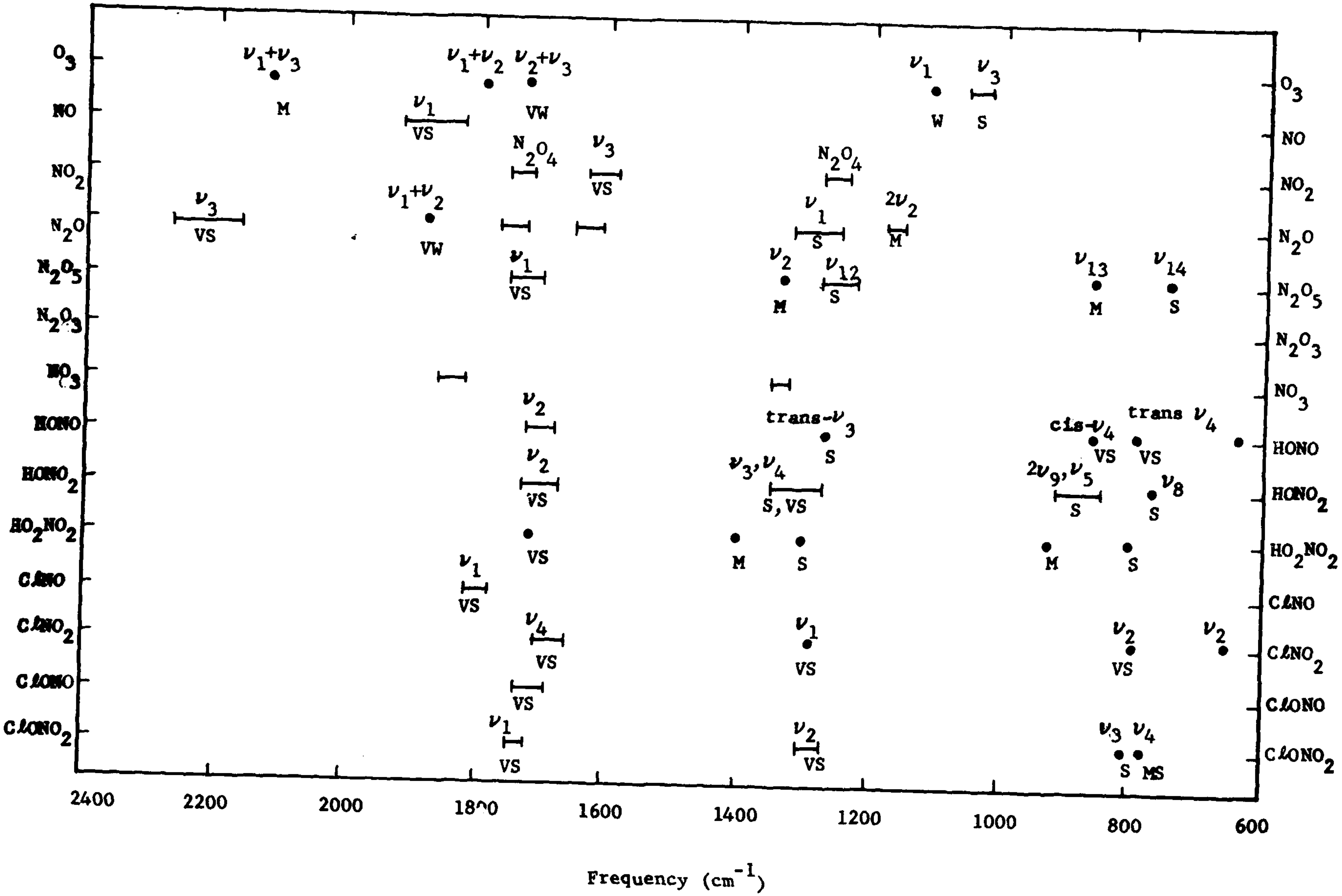


Figure A-2. Summary Chart of Medium Strength and Stronger Bands

ν (cm^{-1})	σ (cm^2/molecule) $\Delta\nu$ = 2.8 cm^{-1}	ν (cm^{-1})	σ (cm^2/molecule) $\Delta\nu$ = 1.0 cm^{-1}
1950	1.30×10^{-21}	1950	0.44×10^{-21}
1945	2.22	1945	0.94
1940	3.23	1940	1.55
1935	4.24	1935	2.23
1930	5.41	1930	3.06
1925	6.78	1930	4.17
1920	7.49	1920	4.91
1915	8.03	1915	6.17
1910	8.17	1910	6.95
1905	8.32	1905	7.29
1900	7.63	1900	7.13
1895	7.46	1895	6.28
1890	6.58	1890	5.25
1885	4.21	1885	3.81
1880	1.99	1880	0.04
1876(Q)	7.53	1876(Q)	10.18
1870	3.81	1870	0.49
1865	7.04	1865	5.44
1860	8.68	1860	6.61
1855	6.47	1855	6.72
1850	7.55	1850	6.01
1845	10.3	1845	6.01
1840	7.07	1840	4.49
1835	6.83	1835	4.04
1830	6.41	1830	3.97
1825	6.02	1825	4.22
1820	4.46	1820	2.60
1815	3.48	1815	2.12
1810	2.51	1810	1.60
1805	2.51	1805	1.96
1800	2.27	1800	1.44

A.2.2 Nitrogen Dioxide

The data presented for the ν_3 band was taken from Goldman et al., (1975), and corresponds to a resolution of about 10 cm^{-1}.

ν (cm^{-1})	$S°/d$ (cm^{-1}-atm^{-1})	σ (cm^2/molecule)
1650	3.0	0.128×10^{-18}
1645	7.7	0.330
1640	18.0	0.768
1635	25.0	1.066
1630	31.5	1.343
1625	27.0	1.151
1620	17.5	0.746
1615	15.4	0.659
1610	19.0	0.811
1605	23.0	0.981
1600	25.0	1.066
1595	23.0	0.984
1590	18.0	0.768
1585	12.5	0.533
1580	8.7	0.373
1575	5.7	0.245
1570	3.5	0.149

A.2.3 Nitrogen Trioxide Radical

Nitrogen Trioxide is a free radical intermediate in the N_2O_5 - O_3 system and was also observed in room temperature decomposition of $ClONO_2$. The data presented for the 1360 cm^{-1} band was extracted from Cramarossa and Johnston (1965), and corresponds to a resolution of about 3 cm^{-1}.

ν (cm^{-1})	σ (cm^2/molecule)
1410	0.029×10^{-18}
1400	0.038
1390	0.054

ν (cm^{-1})	σ (cm^2/molecule)
1380	0.072
1370	0.098
1360	0.150
1350	0.088
1340	0.060
1330	0.040
1320	0.022
1310	0.016

A.2.4 Nitrous Pentoxide

The data presented for the ν_1 band was extracted from Nightingale et al., (1954) and the ν_2 cross-section data given below. The data presented for the ν_2 and ν_{12} bands was extracted from Graham (1975) and corresponds to a resolution of 5.10 cm^{-1}.

ν (cm^{-1})	σ (cm^2/molecule)	ν (cm^{-1})	σ (cm^2/molecule)	ν (cm^{-1})	σ (cm^2/molecule)
1780	0.338×10^{-18}	1370	0.065×10^{-18}	1260	0.50×10^{-18}
1770	0.595	1365	0.080	1255	1.30
1760	0.910	1360	0.097	1250	1.52
1750	1.295	1355	0.113	1245	1.73
1740	1.824	1350	0.127	1240	1.58
1730	2.380	1345	0.142	1235	1.01
1720	2.169	1340	0.149	1230	0.24
1710	1.546	1335	0.135		
1700	1.082	1330	0.111		
1690	0.732	1325	0.089	1252	1.55
1680	0.393	1320	0.068	1246	1.75

A.2.6 Chlorine Nitrate

The data presented for the ν_1 and ν_2 bands was taken from Graham et al., (1977), and corresponds to a resolution of about 0.0625 cm^{-1}. The cross-section values are independent of resolution and pressure.

ν (cm^{-1})	σ (cm^2/molecule)	ν (cm^{-1})	σ (cm^2/molecule)
1760	0.186×10^{-18}	1310	0.186×10^{-18}
1755	0.335	1305	0.595
1750	0.744	1300	1.116
1745	1.339	1295	0.476
1740	0.893	1290	0.707
1735	1.041	1285	0.986
1730	1.320	1280	0.558
1725	1.004	1275	0.186
1720	0.707	1270	0.074
1715	0.446		
1710	0.242		
1731(P)	1.361	1286(P)	1.004
1738(Q)	1.153	1292(Q)	1.897
1744(R)	1.413	1300(R)	1.116

A.2.7 Ozone

The data presented for the ν_3 band was extracted from Pitts et al., (1976) and corresponds to a resolution of about 1.3 cm^{-1}.

ν (cm^{-1})	σ (cm^2/molecule)
1065	0.0614×10^{-18}
1060	0.1235
1055	0.1717

A.2.5 Nitric Acid

The data presented for the ν_2 and ν_3 bands was taken from Goldman et al., (1971), and corresponds to a resolution of ~ 0.5 cm^{-1}.

ν (cm^{-1})	S°/d (cm^{-1}-atm^{-1})	σ (cm^2/molecule)
1735	9.420	0.4017×10^{-18}
1730	17.68	0.7539
1725	24.79	1.057
1720	25.84	1.102
1715	26.99	1.151
1710	21.09	0.899
1705	23.22	0.990
1700	23.58	1.005
1695	23.31	0.994
1690	19.83	0.845
1685	14.12	0.602
1680	8.803	0.375
1350	8.716	0.3717
1345	14.87	0.6340
1340	17.87	0.7620
1335	16.42	0.7001
1330	16.82	0.7172
1325	21.32	0.9091
1320	21.68	0.9244
1315	23.09	0.9845
1310	21.51	0.9172
1305	18.00	0.7675
1300	13.74	0.5859
1395	10.51	0.4481
1290	8.759	0.3735

ν (cm^{-1})	σ (cm^2/molecule)
1050	0.1376
1045	0.0530
1040	0.0793
1035	0.1200
1030	0.1306
1025	0.1323
1020	0.1253
1015	0.0956
1010	0.0819
1005	0.0716
1000	0.0530

APPENDIX B

COMPUTER SIMULATION OF NO_z THERMAL CONVERSION IN THE STRATOSPHERE

The computer code was developed to evaluate the performance of ideal thermal converters operating on stratospheric gas samples. The intent was to follow the temporal evolution of the sample to determine the decomposition paths and the significance of the final product abundances. The model included most of the major odd-nitrogen compounds and other important stratospheric constituents. The constituent set was extended until it included chlorine nitrate and chlorine oxide. At that point, the set was fixed because further expansion would have involved the entire family of chlorine compounds and their associated reactions. Such an expansion would have been beyond the scope of this study. Table B-1 contains a list of the molecules considered and the abundances used as the initial conditions for the computer code. In all, nineteen constituents were used together with forty reactions among them. Reactions with unknown products were ignored. Also, an NO_2 photolysis reaction was included but not used for this computation.

The evolution of the abundances was determined using the EPISODE version of the GEARS code. EPISODE is a computer algorithm for the solution of ordinary differential equations. Reaction rates were taken from the literature (principally the review by Hampson and Garvin, 1978). When both forward and backward rates were known, they were used directly. Otherwise, the equilibrium constant was evaluated and used to determine the "missing" rate (cf; Section 3.1).

The output format begins with a listing of the reactions and their evaluated rates at the initial conditions of temperature and pressure. The third body or "M" dependence is included in the reaction rates both as a computational convenience and as an aid to highlighting the significant rates. The temporal evolution of each constituent then follows.

TABLE B-1. MOLECULAR NUMBER DENSITIES USED FOR SAMPLE MODELING WITHIN INSTRUMENTATION

MOLECULE	T(K) Pmb(Torr) H(km)	217 120 mb(91) 15	217 55(42) 20	222 25(19) 25	227 12(9.1) 30	237 6(4.6) 35	251 2.6(2.0) 40
O_3		2.5×10^{12}	4.5×10^{12}	4.2×10^{12}	2.5×10^{12}	1.3×10^{12}	6.0×10^{11}
NO		5.0×10^{9}	1.5×10^{9}	7.0×10^{8}	4.5×10^{8}	5.5×10^{8}	7.0×10^{8}
NO_2		4.5×10^{9}	8.0×10^{9}	6.5×10^{9}	4.2×10^{9}	2.2×10^{9}	7.0×10^{8}
N_2O_5		1.0×10^{7}	4.0×10^{8}	7.0×10^{8}	4.0×10^{8}	5.5×10^{7}	3.5×10^{6}
HNO_3		1.5×10^{9}	4.0×10^{9}	2.0×10^{9}	4.0×10^{8}	4.9×10^{7}	
$ClONO_2$		5.0×10^{7}(est)	1.0×10^{8}	4.0×10^{8}	2.0×10^{8}	4.0×10^{7}	
HO_2NO_2		2.0×10^{9}	4.0×10^{9}	3.5×10^{9}	1.5×10^{9}	2.3×10^{8}	
HO_2		1.5×10^{7}	2.0×10^{7}	2.3×10^{7}	2.5×10^{7}	1.7×10^{7}	8.0×10^{6}
NO_3		2.0×10^{4}	5.0×10^{5}	2.0×10^{6}	3.0×10^{6}	2.0×10^{6}	1.0×10^{6}
O_2		8.2×10^{17}	3.8×10^{17}	1.7×10^{17}	7.8×10^{16}	3.8×10^{16}	
HO		2.0×10^{6}	1.0×10^{6}	1.5×10^{6}	3.0×10^{6}	5.0×10^{6}	1.0×10^{7}
H_2O		7.3×10^{12}	3.8×10^{12}	1.9×10^{12}	1.2×10^{12}	5.3×10^{11}	
O		1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	
H		1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	
H_2		1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	
H_2O_2		8.5×10^{8}	1.3×10^{9}	1.8×10^{9}	1.2×10^{9}	2.8×10^{8}	4.0×10^{7}
HNO		1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	1.0×10^{6}	
HNO_2		6.0×10^{6}	1.0×10^{6}	8.0×10^{5}	8.0×10^{5}	7.0×10^{5}	6.0×10^{5}
ClO		2.0×10^{7}(est)	3.5×10^{7}	5.7×10^{7}	4.5×10^{7}	5.0×10^{7}	

T=250 K, H=15 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.94D-05	6.07D-13
2	2*NO3 >>> 2*NO2 + O2	4.71D-17	7.46D-62
3	NO2 + NO3 >>> NO2 + NO + O2	4.21D-15	1.19D-34
4	NO3 + NO >>> 2*NO2	1.90D-11	3.29D-32
5	NO + O3 >>> NO2 + O2	6.36D-15	1.08D-56
6	NO2 + O3 >>> NO3 + O2	6.65D-18	8.33D-39
7	HNO3 + M >>> HO + NO2 + M	2.58D-27	1.18D-11
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.80D-29
9	O + O + M >>> O2 + M	1.29D-14	3.31D-56
10	O + O2 + M >>> O3 + M	2.77D-15	7.76D-12
11	O + O3 >>> 2*O2	1.92D-15	0.0
12	O + NO + M >>> NO2 + M	5.44D-13	4.03D-47
13	O + NO2 >>> NO + O2	5.12D-12	6.27D-53
14	O + NO2 + M >>> NO3 + M	3.39D-13	2.72D-23
15	HO + HO >>> H2O + O	1.09D-12	9.77D-27
16	O2 + 2*NO >>> 2*NO2	2.75D-38	3.88D-35
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	7.73D-25
19	O + HO2 >>> HO + O2	1.08D-11	5.45D-60
20	O2 + H + M >>> HO2 + M	1.34D-13	1.71D-30
21	O3 + H >>> HO + O2	1.27D-11	0.0
22	O3 + HO >>> HO2 + O2	2.75D-14	1.04D-48
23	O3 + HO2 >>> HO + 2*O2	4.45D-16	2.41D-68
24	H + HO + M >>> H2O + M	2.72D-12	0.0
25	H + HO2 >>> 2*HO	9.40D-12	1.62D-46
26	H + HO2 >>> H2 + O2	1.04D-11	2.55D-61
27	H + H2O >>> H2 + HO	2.34D-28	1.14D-15
28	H + H2O2 >>> H2 + HO2	8.36D-15	5.62D-29
29	H + H2O2 >>> HO + H2O	1.09D-14	1.35D-75

30	2*HO + M >>> H2O2 + M	1.55D-12	4.17D-31
31	HO + HO2 >>> H2O + O2	1.12D-11	3.89D-74
32	2*HO2 >>> H2O2 + O2	2.30D-12	8.58D-49
33	HO2 + H2O >>> H2O2 + HO	1.02D-39	5.49D-13
34	NO + H + M >>> HNO + M	8.45D-14	1.32D-32
35	NO + HO >>> NO2 + H	3.05D-38	3.01D-11
36	NO + HO + M >>> HNO2 + M	1.11D-11	4.21D-28
37	NO + HO2 >>> NO2 + HO	1.65D-13	7.47D-21
38	H + H + M >>> H2 + M	3.39D-15	0.0
39	HNO4 + M >>> HO2 + NO2 + M	3.64D-05	6.73D-13
40	CLNO3 + M >>> CLO + NO2 + M	1.57D-06	6.11D-13

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	1.0000D 07	4.5000D 09	2.0000D 04	5.0000D 09	2.5000D 12	8.2000D 17	1.5000D 09	2.0000D 06	7.3000D 12
0.20	1.0000D 07	4.5160D 09	3.4990D 04	4.9840D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.9360D 06	7.3000D 12
0.40	1.0000D 07	4.5320D 09	4.9740D 04	4.9680D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.8750D 06	7.3000D 12
0.60	1.0000D 07	4.5470D 09	6.4250D 04	4.9520D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.8150D 06	7.3000D 12
0.80	1.0000D 07	4.5630D 09	7.8550D 04	4.9370D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.7580D 06	7.3000D 12
1.00	1.0000D 07	4.5790D 09	9.2620D 04	4.9210D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.7020D 06	7.3000D 12
1.20	1.0000D 07	4.5940D 09	1.0650D 05	4.9050D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.6490D 06	7.3000D 12
1.40	1.0000D 07	4.6100D 09	1.2010D 05	4.8900D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.5970D 06	7.3000D 12
1.60	1.0000D 07	4.6250D 09	1.3360D 05	4.8740D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.5470D 06	7.3000D 12
1.80	1.0000D 07	4.6410D 09	1.4680D 05	4.8590D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.4990D 06	7.3000D 12
2.00	1.0000D 07	4.6560D 09	1.5990D 05	4.8430D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.4530D 06	7.3000D 12
2.20	1.0000D 07	4.6710D 09	1.7280D 05	4.8280D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.4080D 06	7.3000D 12
2.40	1.0000D 07	4.6870D 09	1.8550D 05	4.8130D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.3650D 06	7.3000D 12
2.60	1.0000D 07	4.7020D 09	1.9800D 05	4.7970D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.3230D 06	7.3000D 12
2.80	1.0000D 07	4.7170D 09	2.1030D 05	4.7820D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.2830D 06	7.3000D 12
3.00	1.0000D 07	4.7320D 09	2.2250D 05	4.7670D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.2440D 06	7.3000D 12
3.20	1.0000D 07	4.7470D 09	2.3450D 05	4.7520D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.2060D 06	7.3000D 12
3.40	1.0000D 07	4.7620D 09	2.4640D 05	4.7370D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.1700D 06	7.3000D 12
3.60	1.0000D 07	4.7770D 09	2.5810D 05	4.7220D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.1350D 06	7.3000D 12
3.80	1.0000D 07	4.7920D 09	2.6960D 05	4.7070D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.1020D 06	7.3000D 12
4.00	1.0000D 07	4.8070D 09	2.8100D 05	4.6920D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.0690D 06	7.3000D 12
4.20	1.0000D 07	4.8220D 09	2.9230D 05	4.6770D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.0380D 06	7.3000D 12
4.40	1.0000D 07	4.8370D 09	3.0340D 05	4.6620D 09	2.5000D 12	8.2000D 17	1.5000D 09	1.0070D 06	7.3000D 12
4.60	1.0000D 07	4.8520D 09	3.1430D 05	4.6470D 09	2.5000D 12	8.2000D 17	1.5000D 09	9.7820D 05	7.3000D 12
4.80	1.0000D 07	4.8670D 09	3.2520D 05	4.6320D 09	2.5000D 12	8.2000D 17	1.5000D 09	9.4990D 05	7.3000D 12
5.00	1.0000D 07	4.8810D 09	3.3590D 05	4.6180D 09	2.5000D 12	8.2000D 17	1.5000D 09	9.2270D 05	7.3000D 12
5.20	1.0000D 07	4.8960D 09	3.4650D 05	4.6030D 09	2.5000D 12	8.2000D 17	1.5000D 09	8.9640D 05	7.3000D 12
5.40	1.0000D 07	4.9100D 09	3.5690D 05	4.5880D 09	2.5000D 12	8.2000D 17	1.5000D 09	8.7100D 05	7.3000D 12
5.60	1.0000D 07	4.9250D 09	3.6730D 05	4.5740D 09	2.5000D 12	8.2000D 17	1.5000D 09	8.4650D 05	7.3000D 12
5.80	1.0000D 07	4.9390D 09	3.7750D 05	4.5590D 09	2.5000D 12	8.2000D 17	1.5000D 09	8.2290D 05	7.3000D 12
6.00	1.0000D 07	4.9540D 09	3.8760D 05	4.5450D 09	2.5000D 12	8.2000D 17	1.5000D 09	8.0010D 05	7.3000D 12
6.20	1.0000D 07	4.9680D 09	3.9760D 05	4.5300D 09	2.5000D 12	8.2000D 17	1.5000D 09	7.7800D 05	7.3000D 12
6.40	1.0000D 07	4.9830D 09	4.0750D 05	4.5160D 09	2.5000D 12	8.2000D 17	1.5000D 09	7.5680D 05	7.3000D 12
6.60	1.0000D 07	4.9970D 09	4.1720D 05	4.5010D 09	2.5000D 12	8.2000D 17	1.5000D 09	7.3620D 05	7.3000D 12
6.80	1.0000D 07	5.0110D 09	4.2690D 05	4.4870D 09	2.4990D 12	8.2000D 17	1.5000D 09	7.1640D 05	7.3000D 12
7.00	1.0000D 07	5.0250D 09	4.3650D 05	4.4730D 09	2.4990D 12	8.2000D 17	1.5000D 09	6.9730D 05	7.3000D 12
7.20	1.0000D 07	5.0400D 09	4.4600D 05	4.4590D 09	2.4990D 12	8.2000D 17	1.5000D 09	6.7890D 05	7.3000D 12
7.40	1.0000D 07	5.0540D 09	4.5530D 05	4.4450D 09	2.4990D 12	8.2000D 17	1.5000D 09	6.6100D 05	7.3000D 12
7.60	1.0000D 07	5.0680D 09	4.6460D 05	4.4300D 09	2.4990D 12	8.2000D 17	1.5000D 09	6.4380D 05	7.3000D 12
7.80	1.0000D 07	5.0820D 09	4.7380D 05	4.4160D 09	2.4990D 12	8.2000D 17	1.5010D 09	6.2720D 05	7.3000D 12
8.00	1.0000D 07	5.0960D 09	4.8290D 05	4.4020D 09	2.4990D 12	8.2000D 17	1.5010D 09	6.1120D 05	7.3000D 12
8.20	1.0010D 07	5.1100D 09	4.9190D 05	4.3880D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.9570D 05	7.3000D 12
8.40	1.0010D 07	5.1240D 09	5.0090D 05	4.3740D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.8080D 05	7.3000D 12
8.60	1.0010D 07	5.1380D 09	5.0970D 05	4.3600D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.6640D 05	7.3000D 12
8.80	1.0010D 07	5.1510D 09	5.1850D 05	4.3470D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.5250D 05	7.3000D 12
9.00	1.0010D 07	5.1650D 09	5.2720D 05	4.3330D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.3900D 05	7.3000D 12
9.20	1.0010D 07	5.1790D 09	5.3580D 05	4.3190D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.2610D 05	7.3000D 12
9.40	1.0010D 07	5.1930D 09	5.4430D 05	4.3050D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.1350D 05	7.3000D 12
9.60	1.0010D 07	5.2060D 09	5.5280D 05	4.2920D 09	2.4990D 12	8.2000D 17	1.5010D 09	5.0140D 05	7.3000D 12
9.80	1.0010D 07	5.2200D 09	5.6120D 05	4.2780D 09	2.4990D 12	8.2000D 17	1.5010D 09	4.8980D 05	7.3000D 12
10.00	1.0010D 07	5.2330D 09	5.6960D 05	4.2640D 09	2.4990D 12	8.2000D 17	1.5010D 09	4.7850D 05	7.3000D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	1.5000D 07	8.5000D 08	1.0000D 06	6.0000D 06	2.0000D 09	5.0000D 07
0.20	1.0340D-02	2.0150D-08	1.0000D 06	1.6030D 07	8.5000D 08	1.0000D 06	6.0220D 06	2.0000D 09	5.0010D 07
0.40	1.0230D-02	1.9500D-08	1.0000D 06	1.6050D 07	8.5000D 08	1.0000D 06	6.0430D 06	2.0000D 09	5.0020D 07
0.60	1.0120D-02	1.8890D-08	1.0000D 06	1.6070D 07	8.5000D 08	1.0000D 06	6.0630D 06	2.0000D 09	5.0030D 07
0.80	1.0020D-02	1.8290D-08	1.0000D 06	1.6100D 07	8.5000D 08	1.0000D 06	6.0830D 06	2.0000D 09	5.0040D 07
1.00	9.9330D-03	1.7710D-08	1.0000D 06	1.6120D 07	8.5000D 08	1.0000D 06	6.1020D 06	2.0000D 09	5.0060D 07
1.20	9.8470D-03	1.7150D-08	1.0000D 06	1.6140D 07	8.5000D 08	1.0000D 06	6.1200D 06	2.0000D 09	5.0070D 07
1.40	9.7670D-03	1.6620D-08	1.0000D 06	1.6160D 07	8.5000D 08	1.0000D 06	6.1380D 06	2.0000D 09	5.0080D 07
1.60	9.6920D-03	1.6100D-08	1.0000D 06	1.6180D 07	8.5000D 08	1.0000D 06	6.1550D 06	2.0000D 09	5.0090D 07
1.80	9.6210D-03	1.5600D-08	1.0000D 06	1.6200D 07	8.5000D 08	1.0000D 06	6.1710D 06	2.0000D 09	5.0100D 07
2.00	9.5560D-03	1.5120D-08	1.0000D 06	1.6220D 07	8.5000D 08	1.0000D 06	6.1870D 06	2.0000D 09	5.0110D 07
2.20	9.4940D-03	1.4650D-08	1.0000D 06	1.6240D 07	8.5000D 08	1.0000D 06	6.2020D 06	2.0000D 09	5.0120D 07
2.40	9.4370D-03	1.4200D-08	1.0000D 06	1.6250D 07	8.5000D 08	1.0000D 06	6.2170D 06	2.0000D 09	5.0130D 07
2.60	9.3830D-03	1.3770D-08	1.0000D 06	1.6270D 07	8.5000D 08	1.0000D 06	6.2320D 06	2.0000D 09	5.0150D 07
2.80	9.3330D-03	1.3350D-08	1.0000D 06	1.6280D 07	8.5000D 08	1.0000D 06	6.2460D 06	2.0000D 09	5.0160D 07
3.00	9.2860D-03	1.2940D-08	1.0000D 06	1.6300D 07	8.5000D 08	1.0000D 06	6.2590D 06	2.0000D 09	5.0170D 07
3.20	9.2420D-03	1.2550D-08	1.0000D 06	1.6310D 07	8.5000D 08	1.0000D 06	6.2720D 06	2.0000D 09	5.0180D 07
3.40	9.2010D-03	1.2180D-08	1.0000D 06	1.6330D 07	8.5000D 08	1.0000D 06	6.2840D 06	2.0000D 09	5.0190D 07
3.60	9.1620D-03	1.1810D-08	1.0000D 06	1.6340D 07	8.5000D 08	1.0000D 06	6.2970D 06	2.0000D 09	5.0200D 07
3.80	9.1260D-03	1.1460D-08	1.0000D 06	1.6360D 07	8.5000D 08	1.0000D 06	6.3080D 06	2.0000D 09	5.0210D 07
4.00	9.0920D-03	1.1120D-08	1.0000D 06	1.6370D 07	8.5000D 08	1.0000D 06	6.3200D 06	2.0000D 09	5.0230D 07
4.20	9.0600D-03	1.0800D-08	1.0000D 06	1.6380D 07	8.5000D 08	1.0000D 06	6.3310D 06	2.0000D 09	5.0240D 07
4.40	9.0310D-03	1.0480D-08	1.0000D 06	1.6390D 07	8.5000D 08	1.0000D 06	6.3410D 06	2.0000D 09	5.0250D 07
4.60	9.0030D-03	1.0180D-08	1.0000D 06	1.6400D 07	8.5000D 08	1.0000D 06	6.3510D 06	2.0000D 09	5.0260D 07
4.80	8.9770D-03	9.8830D-09	1.0000D 06	1.6410D 07	8.5000D 08	1.0000D 06	6.3610D 06	2.0000D 09	5.0270D 07
5.00	8.9520D-03	9.6000D-09	1.0000D 06	1.6420D 07	8.5000D 08	1.0000D 06	6.3710D 06	2.0000D 09	5.0280D 07
5.20	8.9290D-03	9.3260D-09	1.0000D 06	1.6430D 07	8.5000D 08	1.0000D 06	6.3800D 06	2.0000D 09	5.0300D 07
5.40	8.9080D-03	9.0620D-09	1.0000D 06	1.6440D 07	8.5000D 08	1.0000D 06	6.3890D 06	2.0000D 09	5.0310D 07
5.60	8.8870D-03	8.8070D-09	1.0000D 06	1.6450D 07	8.5000D 08	1.0000D 06	6.3980D 06	2.0000D 09	5.0320D 07
5.80	8.8680D-03	8.5610D-09	1.0000D 06	1.6460D 07	8.5000D 08	1.0000D 06	6.4060D 06	2.0000D 09	5.0330D 07
6.00	8.8510D-03	8.3240D-09	1.0000D 06	1.6470D 07	8.5000D 08	1.0000D 06	6.4150D 06	2.0000D 09	5.0340D 07
6.20	8.8340D-03	8.0950D-09	1.0000D 06	1.6480D 07	8.5000D 08	1.0000D 06	6.4230D 06	2.0000D 09	5.0360D 07
6.40	8.8180D-03	7.8730D-09	1.0000D 06	1.6490D 07	8.5000D 08	1.0000D 06	6.4300D 06	2.0000D 09	5.0370D 07
6.60	8.8040D-03	7.6600D-09	1.0000D 06	1.6490D 07	8.5000D 08	1.0000D 06	6.4380D 06	2.0000D 09	5.0380D 07
6.80	8.7900D-03	7.4540D-09	1.0000D 06	1.6500D 07	8.5000D 08	1.0000D 06	6.4450D 06	2.0000D 09	5.0390D 07
7.00	8.7770D-03	7.2550D-09	1.0000D 06	1.6510D 07	8.5000D 08	1.0000D 06	6.4520D 06	2.0000D 09	5.0400D 07
7.20	8.7650D-03	7.0630D-09	1.0000D 06	1.6510D 07	8.5000D 08	1.0000D 06	6.4590D 06	2.0000D 09	5.0420D 07
7.40	8.7530D-03	6.8770D-09	1.0000D 06	1.6520D 07	8.5000D 08	1.0000D 06	6.4660D 06	2.0000D 09	5.0430D 07
7.60	8.7420D-03	6.6980D-09	1.0000D 06	1.6530D 07	8.5000D 08	1.0000D 06	6.4720D 06	2.0000D 09	5.0440D 07
7.80	8.7320D-03	6.5260D-09	1.0000D 06	1.6530D 07	8.5000D 08	1.0000D 06	6.4780D 06	2.0000D 09	5.0450D 07
8.00	8.7230D-03	6.3590D-09	1.0000D 06	1.6540D 07	8.5000D 08	1.0000D 06	6.4840D 06	2.0000D 09	5.0460D 07
8.20	8.7140D-03	6.1980D-09	1.0000D 06	1.6540D 07	8.5000D 08	1.0000D 06	6.4900D 06	2.0000D 09	5.0480D 07
8.40	8.7050D-03	6.0430D-09	1.0000D 06	1.6550D 07	8.5000D 08	1.0000D 06	6.4960D 06	2.0000D 09	5.0490D 07
8.60	8.6970D-03	5.8930D-09	1.0000D 06	1.6550D 07	8.5000D 08	1.0000D 06	6.5010D 06	2.0000D 09	5.0500D 07
8.80	8.6900D-03	5.7480D-09	1.0000D 06	1.6560D 07	8.5000D 08	1.0000D 06	6.5070D 06	2.0000D 09	5.0510D 07
9.00	8.6830D-03	5.6080D-09	1.0000D 06	1.6560D 07	8.5000D 08	1.0000D 06	6.5120D 06	2.0000D 09	5.0520D 07
9.20	8.6760D-03	5.4730D-09	1.0000D 06	1.6560D 07	8.5000D 08	1.0000D 06	6.5170D 06	2.0000D 09	5.0540D 07
9.40	8.6700D-03	5.3430D-09	1.0000D 06	1.6570D 07	8.5000D 08	1.0000D 06	6.5220D 06	2.0000D 09	5.0550D 07
9.60	8.6640D-03	5.2170D-09	1.0000D 06	1.6570D 07	8.5000D 08	1.0000D 06	6.5270D 06	2.0000D 09	5.0560D 07
9.80	8.6580D-03	5.0950D-09	1.0000D 06	1.6580D 07	8.5000D 08	1.0000D 06	6.5320D 06	2.0000D 09	5.0570D 07
10.00	8.6530D-03	4.9780D-09	1.0000D 06	1.6580D 07	8.5000D 08	1.0000D 06	6.5360D 06	2.0000D 09	5.0590D 07

T=300 K, H=15 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.57D-02	2.85D-13
2	2*NO3 >>> 2*NO2 + O2	2.41D-16	1.75D-58
3	NO2 + NO3 >>> NO2 + NO + O2	8.21D-15	4.92D-35
4	NO3 + NO >>> 2*NO2	1.90D-11	6.98D-29
5	NO + O3 >>> NO2 + O2	1.67D-14	2.85D-49
6	NO2 + O3 >>> NO3 + O2	3.41D-17	2.00D-34
7	HNO3 + M >>> HO + NO2 + M	1.92D-20	6.24D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	1.25D-26
9	O + O + M >>> O2 + M	5.91D-15	1.26D-56
10	O + O2 + M >>> O3 + M	1.64D-15	1.32D-08
11	O + O3 >>> 2*O2	8.90D-15	0.0
12	O + NO + M >>> NO2 + M	3.07D-13	1.20D-37
13	O + NO2 >>> NO + O2	6.25D-12	3.73D-46
14	O + NO2 + M >>> NO3 + M	2.83D-13	2.26D-23
15	HO + HO >>> H2O + O	1.57D-12	4.63D-24
16	O2 + 2*NO >>> 2*NO2	1.93D-38	2.26D-31
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.16D-22
19	O + HO2 >>> HO + O2	1.51D-11	8.51D-52
20	O2 + H + M >>> HO2 + M	7.98D-14	6.51D-24
21	O3 + H >>> HO + O2	1.79D-11	1.62D-69
22	O3 + HO >>> HO2 + O2	5.35D-14	8.98D-43
23	O3 + HO2 >>> HO + 2*O2	1.04D-15	1.53D-63
24	H + HO + M >>> H2O + M	1.41D-12	1.14D-74
25	H + HO2 >>> 2*HO	1.77D-11	1.14D-40
26	H + HO2 >>> H2 + O2	1.31D-11	6.80D-53
27	H + H2O >>> H2 + HO	2.18D-25	6.41D-15
28	H + H2O2 >>> H2 + HO2	2.13D-14	2.96D-26
29	H + H2O2 >>> HO + H2O	2.76D-14	2.95D-65

30	2*HO + M >>> H2O2 + M	7.10D-13	5.18D-24
31	HO + HO2 >>> H2O + O2	1.57D-11	1.98D-63
32	2*HO2 >>> H2O2 + O2	3.21D-12	1.98D-42
33	HO2 + H2O >>> H2O2 + HO	6.11D-35	8.57D-13
34	NO + H + M >>> HNO + M	5.77D-14	1.48D-25
35	NO + HO >>> NO2 + H	7.19D-34	4.92D-11
36	NO + HO + M >>> HNO2 + M	4.42D-12	2.48D-21
37	NO + HO2 >>> NO2 + HO	3.66D-13	3.74D-19
38	H + H + M >>> H2 + M	2.93D-15	2.43D-68
39	HNO4 + M >>> HO2 + NO2 + M	2.52D-02	3.02D-13
40	CLNO3 + M >>> CLO + NO2 + M	2.28D-03	3.07D-13

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	1.000D 07	4.500D 09	2.000D 04	5.000D 09	2.500D 12	8.200D 17	1.500D 09	2.000D 06	7.300D 12
0.20	9.969D 06	4.552D 09	1.273D 05	4.958D 09	2.500D 12	8.200D 17	1.500D 09	1.946D 06	7.300D 12
0.40	9.937D 06	4.603D 09	2.334D 05	4.917D 09	2.500D 12	8.200D 17	1.500D 09	1.902D 06	7.300D 12
0.60	9.906D 06	4.654D 09	3.382D 05	4.876D 09	2.500D 12	8.200D 17	1.500D 09	1.868D 06	7.300D 12
0.80	9.875D 06	4.704D 09	4.419D 05	4.836D 09	2.500D 12	8.200D 17	1.500D 09	1.844D 06	7.300D 12
1.00	9.844D 06	4.754D 09	5.446D 05	4.795D 09	2.500D 12	8.200D 17	1.500D 09	1.829D 06	7.300D 12
1.20	9.814D 06	4.804D 09	6.461D 05	4.755D 09	2.500D 12	8.200D 17	1.500D 09	1.822D 06	7.300D 12
1.40	9.783D 06	4.853D 09	7.467D 05	4.716D 09	2.500D 12	8.200D 17	1.500D 09	1.824D 06	7.300D 12
1.60	9.753D 06	4.902D 09	8.463D 05	4.676D 09	2.500D 12	8.200D 17	1.500D 09	1.833D 06	7.300D 12
1.80	9.722D 06	4.951D 09	9.449D 05	4.637D 09	2.500D 12	8.200D 17	1.500D 09	1.850D 06	7.300D 12
2.00	9.692D 06	4.999D 09	1.043D 06	4.599D 09	2.500D 12	8.200D 17	1.500D 09	1.874D 06	7.300D 12
2.20	9.662D 06	5.047D 09	1.140D 06	4.560D 09	2.500D 12	8.200D 17	1.500D 09	1.904D 06	7.300D 12
2.40	9.632D 06	5.094D 09	1.236D 06	4.522D 09	2.500D 12	8.200D 17	1.500D 09	1.941D 06	7.300D 12
2.60	9.602D 06	5.141D 09	1.331D 06	4.485D 09	2.499D 12	8.200D 17	1.500D 09	1.984D 06	7.300D 12
2.80	9.572D 06	5.188D 09	1.425D 06	4.447D 09	2.499D 12	8.200D 17	1.500D 09	2.032D 06	7.300D 12
3.00	9.543D 06	5.234D 09	1.519D 06	4.410D 09	2.499D 12	8.200D 17	1.500D 09	2.086D 06	7.300D 12
3.20	9.513D 06	5.280D 09	1.612D 06	4.373D 09	2.499D 12	8.200D 17	1.500D 09	2.145D 06	7.300D 12
3.40	9.484D 06	5.326D 09	1.705D 06	4.337D 09	2.499D 12	8.200D 17	1.500D 09	2.209D 06	7.300D 12
3.60	9.455D 06	5.371D 09	1.797D 06	4.301D 09	2.499D 12	8.200D 17	1.500D 09	2.277D 06	7.300D 12
3.80	9.426D 06	5.416D 09	1.888D 06	4.265D 09	2.499D 12	8.200D 17	1.500D 09	2.350D 06	7.300D 12
4.00	9.397D 06	5.461D 09	1.979D 06	4.229D 09	2.499D 12	8.200D 17	1.500D 09	2.426D 06	7.300D 12
4.20	9.368D 06	5.505D 09	2.069D 06	4.194D 09	2.499D 12	8.200D 17	1.500D 09	2.506D 06	7.300D 12
4.40	9.339D 06	5.549D 09	2.158D 06	4.159D 09	2.499D 12	8.200D 17	1.500D 09	2.590D 06	7.300D 12
4.60	9.311D 06	5.593D 09	2.247D 06	4.124D 09	2.499D 12	8.200D 17	1.500D 09	2.677D 06	7.300D 12
4.80	9.282D 06	5.636D 09	2.336D 06	4.090D 09	2.499D 12	8.200D 17	1.500D 09	2.767D 06	7.300D 12
5.00	9.254D 06	5.679D 09	2.424D 06	4.056D 09	2.499D 12	8.200D 17	1.500D 09	2.859D 06	7.300D 12
5.20	9.225D 06	5.721D 09	2.512D 06	4.022D 09	2.499D 12	8.200D 17	1.500D 09	2.955D 06	7.300D 12
5.40	9.197D 06	5.764D 09	2.599D 06	3.988D 09	2.499D 12	8.200D 17	1.500D 09	3.053D 06	7.300D 12
5.60	9.169D 06	5.806D 09	2.686D 06	3.955D 09	2.499D 12	8.200D 17	1.500D 09	3.153D 06	7.300D 12
5.80	9.142D 06	5.847D 09	2.772D 06	3.922D 09	2.499D 12	8.200D 17	1.500D 09	3.255D 06	7.300D 12
6.00	9.114D 06	5.889D 09	2.858D 06	3.889D 09	2.499D 12	8.200D 17	1.500D 09	3.359D 06	7.300D 12
6.20	9.086D 06	5.930D 09	2.944D 06	3.857D 09	2.499D 12	8.200D 17	1.500D 09	3.465D 06	7.300D 12
6.40	9.059D 06	5.970D 09	3.030D 06	3.824D 09	2.499D 12	8.200D 17	1.501D 09	3.573D 06	7.300D 12
6.60	9.031D 06	6.011D 09	3.115D 06	3.792D 09	2.499D 12	8.200D 17	1.501D 09	3.682D 06	7.300D 12
6.80	9.004D 06	6.051D 09	3.200D 06	3.761D 09	2.499D 12	8.200D 17	1.501D 09	3.792D 06	7.300D 12
7.00	8.977D 06	6.090D 09	3.284D 06	3.729D 09	2.499D 12	8.200D 17	1.501D 09	3.904D 06	7.300D 12
7.20	8.950D 06	6.130D 09	3.369D 06	3.698D 09	2.499D 12	8.200D 17	1.501D 09	4.016D 06	7.300D 12
7.40	8.923D 06	6.169D 09	3.453D 06	3.667D 09	2.499D 12	8.200D 17	1.501D 09	4.130D 06	7.300D 12
7.60	8.896D 06	6.208D 09	3.537D 06	3.637D 09	2.499D 12	8.200D 17	1.501D 09	4.244D 06	7.300D 12
7.80	8.870D 06	6.246D 09	3.620D 06	3.606D 09	2.499D 12	8.200D 17	1.501D 09	4.360D 06	7.300D 12
8.00	8.843D 06	6.284D 09	3.704D 06	3.576D 09	2.499D 12	8.200D 17	1.501D 09	4.475D 06	7.300D 12
8.20	8.817D 06	6.322D 09	3.787D 06	3.546D 09	2.499D 12	8.200D 17	1.501D 09	4.592D 06	7.300D 12
8.40	8.790D 06	6.360D 09	3.870D 06	3.516D 09	2.499D 12	8.200D 17	1.501D 09	4.708D 06	7.300D 12
8.60	8.764D 06	6.397D 09	3.953D 06	3.487D 09	2.498D 12	8.200D 17	1.501D 09	4.825D 06	7.300D 12
8.80	8.738D 06	6.434D 09	4.036D 06	3.458D 09	2.498D 12	8.200D 17	1.501D 09	4.942D 06	7.300D 12
9.00	8.712D 06	6.471D 09	4.119D 06	3.429D 09	2.498D 12	8.200D 17	1.501D 09	5.060D 06	7.300D 12
9.20	8.686D 06	6.508D 09	4.201D 06	3.400D 09	2.498D 12	8.200D 17	1.501D 09	5.177D 06	7.300D 12
9.40	8.661D 06	6.544D 09	4.284D 06	3.372D 09	2.498D 12	8.200D 17	1.501D 09	5.295D 06	7.300D 12
9.60	8.635D 06	6.580D 09	4.366D 06	3.344D 09	2.498D 12	8.200D 17	1.501D 09	5.412D 06	7.300D 12
9.80	8.610D 06	6.615D 09	4.448D 06	3.316D 09	2.498D 12	8.200D 17	1.501D 09	5.529D 06	7.300D 12
10.00	8.584D 06	6.651D 09	4.531D 06	3.288D 09	2.498D 12	8.200D 17	1.501D 09	5.646D 06	7.300D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.000D 06	1.000D 06	1.000D 06	1.500D 07	8.500D 08	1.000D 06	6.000D 06	2.000D 09	5.000D 07
0.20	2.448D 01	2.211D-07	1.000D 06	2.607D 07	8.500D 08	1.000D 06	6.009D 06	1.990D 09	4.998D 07
0.40	2.448D 01	2.161D-07	1.000D 06	3.608D 07	8.500D 08	1.000D 06	6.017D 06	1.980D 09	4.997D 07
0.60	2.448D 01	2.122D-07	1.000D 06	4.603D 07	8.500D 08	1.000D 06	6.025D 06	1.970D 09	4.995D 07
0.80	2.448D 01	2.094D-07	1.000D 06	5.591D 07	8.500D 08	1.000D 06	6.033D 06	1.960D 09	4.993D 07
1.00	2.448D 01	2.077D-07	1.000D 06	6.573D 07	8.500D 08	1.000D 06	6.041D 06	1.950D 09	4.991D 07
1.20	2.448D 01	2.070D-07	1.000D 06	7.548D 07	8.500D 08	1.000D 06	6.049D 06	1.941D 09	4.990D 07
1.40	2.448D 01	2.071D-07	1.000D 06	8.518D 07	8.500D 08	1.000D 06	6.056D 06	1.931D 09	4.988D 07
1.60	2.448D 01	2.082D-07	1.000D 06	9.481D 07	8.500D 08	1.000D 06	6.064D 06	1.921D 09	4.986D 07
1.80	2.448D 01	2.101D-07	1.000D 06	1.044D 08	8.500D 08	1.000D 06	6.071D 06	1.912D 09	4.985D 07
2.00	2.448D 01	2.128D-07	1.000D 06	1.139D 08	8.500D 08	1.000D 06	6.079D 06	1.902D 09	4.983D 07
2.20	2.448D 01	2.163D-07	1.000D 06	1.233D 08	8.500D 08	1.000D 06	6.087D 06	1.892D 09	4.981D 07
2.40	2.447D 01	2.205D-07	1.000D 06	1.327D 08	8.500D 08	1.000D 06	6.094D 06	1.883D 09	4.980D 07
2.60	2.447D 01	2.253D-07	1.000D 06	1.420D 08	8.501D 08	1.000D 06	6.102D 06	1.874D 09	4.978D 07
2.80	2.447D 01	2.308D-07	1.000D 06	1.513D 08	8.501D 08	1.000D 06	6.110D 06	1.864D 09	4.977D 07
3.00	2.447D 01	2.370D-07	1.000D 06	1.605D 08	8.501D 08	1.000D 06	6.118D 06	1.855D 09	4.975D 07
3.20	2.447D 01	2.437D-07	1.000D 06	1.697D 08	8.501D 08	1.000D 06	6.126D 06	1.846D 09	4.973D 07
3.40	2.447D 01	2.509D-07	1.000D 06	1.787D 08	8.501D 08	1.000D 06	6.135D 06	1.836D 09	4.972D 07
3.60	2.447D 01	2.586D-07	1.000D 06	1.878D 08	8.501D 08	1.000D 06	6.143D 06	1.827D 09	4.970D 07
3.80	2.447D 01	2.669D-07	1.000D 06	1.967D 08	8.502D 08	1.000D 06	6.152D 06	1.818D 09	4.968D 07
4.00	2.447D 01	2.755D-07	1.000D 06	2.057D 08	8.502D 08	1.000D 06	6.161D 06	1.809D 09	4.967D 07
4.20	2.447D 01	2.846D-07	1.000D 06	2.145D 08	8.502D 08	1.000D 06	6.170D 06	1.800D 09	4.965D 07
4.40	2.447D 01	2.941D-07	1.000D 06	2.233D 08	8.503D 08	1.000D 06	6.180D 06	1.791D 09	4.964D 07
4.60	2.447D 01	3.040D-07	1.000D 06	2.320D 08	8.503D 08	1.000D 06	6.189D 06	1.782D 09	4.962D 07
4.80	2.448D 01	3.142D-07	1.000D 06	2.407D 08	8.503D 08	1.000D 06	6.199D 06	1.773D 09	4.961D 07
5.00	2.448D 01	3.248D-07	1.000D 06	2.493D 08	8.504D 08	1.000D 06	6.209D 06	1.764D 09	4.959D 07
5.20	2.448D 01	3.356D-07	1.000D 06	2.579D 08	8.504D 08	1.000D 06	6.220D 06	1.756D 09	4.957D 07
5.40	2.448D 01	3.467D-07	1.000D 06	2.664D 08	8.504D 08	1.000D 06	6.230D 06	1.747D 09	4.956D 07
5.60	2.448D 01	3.581D-07	1.000D 06	2.748D 08	8.505D 08	1.000D 06	6.241D 06	1.738D 09	4.954D 07
5.80	2.448D 01	3.697D-07	1.000D 06	2.832D 08	8.505D 08	1.000D 06	6.252D 06	1.730D 09	4.953D 07
6.00	2.448D 01	3.815D-07	1.000D 06	2.916D 08	8.506D 08	1.000D 06	6.264D 06	1.721D 09	4.951D 07
6.20	2.448D 01	3.936D-07	1.000D 06	2.998D 08	8.507D 08	1.000D 06	6.275D 06	1.713D 09	4.950D 07
6.40	2.448D 01	4.058D-07	1.000D 06	3.081D 08	8.507D 08	1.000D 06	6.287D 06	1.704D 09	4.948D 07
6.60	2.448D 01	4.182D-07	1.000D 06	3.162D 08	8.508D 08	1.000D 06	6.299D 06	1.696D 09	4.947D 07
6.80	2.448D 01	4.307D-07	1.000D 06	3.243D 08	8.508D 08	1.000D 06	6.312D 06	1.687D 09	4.945D 07
7.00	2.448D 01	4.434D-07	1.000D 06	3.324D 08	8.509D 08	1.000D 06	6.325D 06	1.679D 09	4.944D 07
7.20	2.448D 01	4.562D-07	1.000D 06	3.404D 08	8.510D 08	1.000D 06	6.338D 06	1.671D 09	4.942D 07
7.40	2.448D 01	4.691D-07	1.000D 06	3.483D 08	8.511D 08	1.000D 06	6.351D 06	1.662D 09	4.941D 07
7.60	2.448D 01	4.821D-07	1.000D 06	3.562D 08	8.511D 08	1.000D 06	6.364D 06	1.654D 09	4.939D 07
7.80	2.448D 01	4.952D-07	1.000D 06	3.641D 08	8.512D 08	1.000D 06	6.378D 06	1.646D 09	4.938D 07
8.00	2.448D 01	5.083D-07	1.000D 06	3.718D 08	8.513D 08	1.000D 06	6.392D 06	1.638D 09	4.936D 07
8.20	2.449D 01	5.215D-07	1.000D 06	3.796D 08	8.514D 08	1.000D 06	6.406D 06	1.630D 09	4.935D 07
8.40	2.449D 01	5.348D-07	1.000D 06	3.872D 08	8.515D 08	1.000D 06	6.421D 06	1.622D 09	4.934D 07
8.60	2.449D 01	5.481D-07	1.000D 06	3.948D 08	8.516D 08	1.000D 06	6.436D 06	1.614D 09	4.932D 07
8.80	2.449D 01	5.614D-07	1.000D 06	4.024D 08	8.517D 08	1.000D 06	6.451D 06	1.606D 09	4.931D 07
9.00	2.449D 01	5.747D-07	1.000D 06	4.099D 08	8.518D 08	1.000D 06	6.466D 06	1.598D 09	4.929D 07
9.20	2.449D 01	5.881D-07	1.000D 06	4.174D 08	8.519D 08	1.000D 06	6.481D 06	1.590D 09	4.928D 07
9.40	2.449D 01	6.014D-07	1.000D 06	4.248D 08	8.520D 08	1.000D 06	6.497D 06	1.582D 09	4.926D 07
9.60	2.449D 01	6.148D-07	1.000D 06	4.321D 08	8.521D 08	1.000D 06	6.513D 06	1.574D 09	4.925D 07
9.80	2.449D 01	6.281D-07	1.000D 06	4.394D 08	8.522D 08	1.000D 06	6.529D 06	1.567D 09	4.924D 07
10.00	2.450D 01	6.414D-07	1.000D 06	4.467D 08	8.524D 08	1.000D 06	6.545D 06	1.559D 09	4.922D 07

T=700 K, H=15 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	2.31D 06	2.37D-14
2	2*NO3 >>> 2*NO2 + O2	2.57D-14	7.44D-49
3	NO2 + NO3 >>> NO2 + NO + O2	5.51D-14	3.97D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.23D-19
5	NO + O3 >>> NO2 + O2	2.65D-13	4.54D-28
6	NO2 + O3 >>> NO3 + O2	3.62D-15	6.56D-22
7	HNO3 + M >>> HO + NO2 + M	1.92D-01	3.21D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	4.74D-19
9	O + O + M >>> O2 + M	4.56D-16	1.43D-19
10	O + O2 + M >>> O3 + M	2.66D-16	1.61D 01
11	O + O3 >>> 2*O2	7.11D-13	8.63D-43
12	O + NO + M >>> NO2 + M	4.33D-14	1.03D-10
13	O + NO2 >>> NO + O2	1.11D-11	8.50D-27
14	O + NO2 + M >>> NO3 + M	1.21D-13	9.70D-24
15	HO + HO >>> H2O + O	4.53D-12	2.04D-16
16	O2 + 2*NO >>> 2*NO2	7.04D-39	9.37D-21
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.11D-15
19	O + HO2 >>> HO + O2	3.91D-11	2.19D-28
20	O2 + H + M >>> HO2 + M	1.32D-14	2.96D-05
21	O3 + H >>> HO + O2	4.78D-11	5.62D-37
22	O3 + HO >>> HO2 + O2	3.59D-13	8.31D-26
23	O3 + HO2 >>> HO + 2*O2	1.18D-14	1.12D-49
24	H + HO + M >>> H2O + M	6.58D-14	1.61D-26
25	H + HO2 >>> 2*HO	1.08D-10	5.87D-24
26	H + HO2 >>> H2 + O2	2.55D-11	8.03D-29
27	H + H2O >>> H2 + HO	6.56D-17	8.90D-13
28	H + H2O2 >>> H2 + HO2	3.06D-13	1.77D-18
29	H + H2O2 >>> HO + H2O	3.98D-13	1.02D-35

30	2*HO + M >>> H2O2 + M	5.48D-14	5.02D-04
31	HO + HO2 >>> H2O + O2	4.06D-11	7.73D-33
32	2*HO2 >>> H2O2 + O2	8.32D-12	3.02D-24
33	HO2 + H2O >>> H2O2 + HO	2.72D-21	3.07D-12
34	NO + H + M >>> HNO + M	1.40D-14	1.05D-05
35	NO + HO >>> NO2 + H	2.23D-21	2.02D-10
36	NO + HO + M >>> HNO2 + M	2.28D-13	2.84D-02
37	NO + HO2 >>> NO2 + HO	3.60D-12	2.68D-14
38	H + H + M >>> H2 + M	1.21D-15	1.01D-24
39	HNO4 + M >>> HO2 + NO2 + M	2.49D 06	2.33D-14
40	CLNO3 + M >>> CLO + NO2 + M	1.80D 06	1.14D-14

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	1.000D 07	4.500D 09	2.000D 04	5.000D 09	2.500D 12	8.200D 17	1.500D 09	2.000D 06	7.300D 12
0.20	2.246D-03	5.185D 09	4.214D 07	6.399D 09	2.226D 12	8.200D 17	1.444D 09	1.012D 09	7.300D 12
0.40	2.972D-03	4.350D 09	6.648D 07	7.264D 09	2.128D 12	8.200D 17	1.389D 09	1.140D 09	7.300D 12
0.60	3.388D-03	3.853D 09	8.558D 07	7.794D 09	2.039D 12	8.200D 17	1.337D 09	1.202D 09	7.300D 12
0.80	3.695D-03	3.552D 09	1.012D 08	8.128D 09	1.957D 12	8.200D 17	1.287D 09	1.254D 09	7.300D 12
1.00	3.961D-03	3.369D 09	1.144D 08	8.346D 09	1.881D 12	8.200D 17	1.239D 09	1.302D 09	7.300D 12
1.20	4.212D-03	3.256D 09	1.258D 08	8.493D 09	1.810D 12	8.200D 17	1.192D 09	1.346D 09	7.300D 12
1.40	4.453D-03	3.187D 09	1.359D 08	8.597D 09	1.745D 12	8.200D 17	1.148D 09	1.386D 09	7.300D 12
1.60	4.685D-03	3.146D 09	1.449D 08	8.672D 09	1.683D 12	8.200D 17	1.105D 09	1.424D 09	7.300D 12
1.80	4.907D-03	3.122D 09	1.529D 08	8.729D 09	1.626D 12	8.200D 17	1.063D 09	1.458D 09	7.300D 12
2.00	5.118D-03	3.108D 09	1.602D 08	8.774D 09	1.572D 12	8.200D 17	1.023D 09	1.489D 09	7.300D 12
2.20	5.318D-03	3.103D 09	1.668D 08	8.811D 09	1.522D 12	8.200D 17	9.849D 08	1.517D 09	7.300D 12
2.40	5.505D-03	3.101D 09	1.727D 08	8.843D 09	1.474D 12	8.200D 17	9.480D 08	1.543D 09	7.300D 12
2.60	5.680D-03	3.103D 09	1.781D 08	8.870D 09	1.429D 12	8.200D 17	9.125D 08	1.566D 09	7.300D 12
2.80	5.842D-03	3.107D 09	1.829D 08	8.895D 09	1.387D 12	8.200D 17	8.784D 08	1.587D 09	7.300D 12
3.00	5.992D-03	3.113D 09	1.873D 08	8.917D 09	1.347D 12	8.200D 17	8.455D 08	1.605D 09	7.300D 12
3.20	6.130D-03	3.119D 09	1.912D 08	8.938D 09	1.309D 12	8.200D 17	8.139D 08	1.622D 09	7.300D 12
3.40	6.257D-03	3.126D 09	1.948D 08	8.958D 09	1.273D 12	8.200D 17	7.835D 08	1.637D 09	7.300D 12
3.60	6.372D-03	3.133D 09	1.979D 08	8.976D 09	1.239D 12	8.200D 17	7.542D 08	1.649D 09	7.300D 12
3.80	6.477D-03	3.140D 09	2.007D 08	8.994D 09	1.206D 12	8.200D 17	7.261D 08	1.661D 09	7.300D 12
4.00	6.571D-03	3.147D 09	2.032D 08	9.011D 09	1.175D 12	8.200D 17	6.990D 08	1.670D 09	7.300D 12
4.20	6.656D-03	3.154D 09	2.053D 08	9.027D 09	1.146D 12	8.200D 17	6.729D 08	1.678D 09	7.300D 12
4.40	6.731D-03	3.161D 09	2.072D 08	9.043D 09	1.118D 12	8.200D 17	6.479D 08	1.685D 09	7.300D 12
4.60	6.798D-03	3.168D 09	2.088D 08	9.058D 09	1.091D 12	8.200D 17	6.237D 08	1.691D 09	7.300D 12
4.80	6.856D-03	3.175D 09	2.101D 08	9.072D 09	1.065D 12	8.200D 17	6.005D 08	1.695D 09	7.300D 12
5.00	6.907D-03	3.182D 09	2.112D 08	9.086D 09	1.041D 12	8.200D 17	5.782D 08	1.698D 09	7.300D 12
5.20	6.950D-03	3.188D 09	2.121D 08	9.100D 09	1.017D 12	8.200D 17	5.567D 08	1.700D 09	7.300D 12
5.40	6.986D-03	3.194D 09	2.128D 08	9.113D 09	9.946D 11	8.200D 17	5.360D 08	1.702D 09	7.300D 12
5.60	7.015D-03	3.201D 09	2.133D 08	9.125D 09	9.729D 11	8.200D 17	5.161D 08	1.702D 09	7.300D 12
5.80	7.038D-03	3.206D 09	2.136D 08	9.138D 09	9.522D 11	8.200D 17	4.970D 08	1.701D 09	7.300D 12
6.00	7.056D-03	3.212D 09	2.137D 08	9.150D 09	9.322D 11	8.200D 17	4.786D 08	1.700D 09	7.300D 12
6.20	7.067D-03	3.218D 09	2.137D 08	9.161D 09	9.130D 11	8.200D 17	4.608D 08	1.698D 09	7.300D 12
6.40	7.074D-03	3.223D 09	2.135D 08	9.172D 09	8.945D 11	8.200D 17	4.438D 08	1.696D 09	7.300D 12
6.60	7.075D-03	3.228D 09	2.132D 08	9.183D 09	8.767D 11	8.200D 17	4.274D 08	1.692D 09	7.300D 12
6.80	7.072D-03	3.234D 09	2.128D 08	9.194D 09	8.596D 11	8.200D 17	4.116D 08	1.689D 09	7.300D 12
7.00	7.065D-03	3.238D 09	2.123D 08	9.204D 09	8.430D 11	8.200D 17	3.964D 08	1.685D 09	7.300D 12
7.20	7.054D-03	3.243D 09	2.116D 08	9.214D 09	8.271D 11	8.200D 17	3.818D 08	1.680D 09	7.300D 12
7.40	7.039D-03	3.248D 09	2.109D 08	9.224D 09	8.117D 11	8.200D 17	3.677D 08	1.675D 09	7.300D 12
7.60	7.020D-03	3.252D 09	2.100D 08	9.233D 09	7.968D 11	8.200D 17	3.541D 08	1.669D 09	7.300D 12
7.80	6.998D-03	3.257D 09	2.091D 08	9.242D 09	7.824D 11	8.200D 17	3.411D 08	1.663D 09	7.300D 12
8.00	6.973D-03	3.261D 09	2.081D 08	9.251D 09	7.685D 11	8.200D 17	3.286D 08	1.657D 09	7.300D 12
8.20	6.945D-03	3.265D 09	2.070D 08	9.260D 09	7.551D 11	8.200D 17	3.165D 08	1.651D 09	7.300D 12
8.40	6.914D-03	3.269D 09	2.058D 08	9.268D 09	7.421D 11	8.200D 17	3.049D 08	1.644D 09	7.300D 12
8.60	6.881D-03	3.272D 09	2.046D 08	9.276D 09	7.295D 11	8.200D 17	2.937D 08	1.637D 09	7.300D 12
8.80	6.846D-03	3.276D 09	2.033D 08	9.284D 09	7.173D 11	8.200D 17	2.830D 08	1.630D 09	7.300D 12
9.00	6.809D-03	3.279D 09	2.020D 08	9.292D 09	7.054D 11	8.200D 17	2.726D 08	1.622D 09	7.300D 12
9.20	6.769D-03	3.283D 09	2.006D 08	9.299D 09	6.939D 11	8.200D 17	2.627D 08	1.615D 09	7.300D 12
9.40	6.728D-03	3.286D 09	1.992D 08	9.306D 09	6.828D 11	8.200D 17	2.531D 08	1.607D 09	7.300D 12
9.60	6.685D-03	3.289D 09	1.978D 08	9.314D 09	6.720D 11	8.200D 17	2.439D 08	1.599D 09	7.300D 12
9.80	6.641D-03	3.292D 09	1.963D 08	9.320D 09	6.615D 11	8.200D 17	2.350D 08	1.591D 09	7.300D 12
10.00	6.595D-03	3.295D 09	1.947D 08	9.327D 09	6.513D 11	8.200D 17	2.264D 08	1.583D 09	7.300D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	1.5000D 07	8.5000D 08	1.0000D 06	6.0000D 06	2.0000D 09	5.0000D 07
0.20	1.6310D 11	5.4730D 05	1.0020D 06	1.1370D 09	8.5290D 08	1.0000D 06	6.1500D 06	5.5110D-02	2.2890D-03
0.40	1.5600D 11	5.9040D 05	1.0060D 06	1.1310D 09	8.5440D 08	1.0000D 06	6.4570D 06	4.5990D-02	1.9200D-03
0.60	1.4950D 11	5.9640D 05	1.0090D 06	1.1840D 09	8.5590D 08	1.0000D 06	6.8230D 06	4.2630D-02	1.7010D-03
0.80	1.4350D 11	5.9760D 05	1.0130D 06	1.2370D 09	8.5760D 08	1.0000D 06	7.2310D 06	4.1060D-02	1.5680D-03
1.00	1.3800D 11	5.9660D 05	1.0160D 06	1.2860D 09	8.5950D 08	1.0000D 06	7.6700D 06	4.0490D-02	1.4870D-03
1.20	1.3280D 11	5.9390D 05	1.0200D 06	1.3310D 09	8.6160D 08	1.0000D 06	8.1350D 06	4.0530D-02	1.4380D-03
1.40	1.2800D 11	5.8990D 05	1.0240D 06	1.3730D 09	8.6390D 08	1.0000D 06	8.6210D 06	4.0910D-02	1.4070D-03
1.60	1.2350D 11	5.8460D 05	1.0280D 06	1.4120D 09	8.6630D 08	1.0000D 06	9.1250D 06	4.1510D-02	1.3890D-03
1.80	1.1930D 11	5.7840D 05	1.0320D 06	1.4470D 09	8.6890D 08	1.0000D 06	9.6450D 06	4.2210D-02	1.3780D-03
2.00	1.1540D 11	5.7140D 05	1.0360D 06	1.4790D 09	8.7160D 08	1.0000D 06	1.0180D 07	4.2970D-02	1.3720D-03
2.20	1.1170D 11	5.6370D 05	1.0400D 06	1.5080D 09	8.7440D 08	1.0000D 06	1.0720D 07	4.3730D-02	1.3700D-03
2.40	1.0820D 11	5.5550D 05	1.0440D 06	1.5340D 09	8.7740D 08	1.0000D 06	1.1280D 07	4.4480D-02	1.3690D-03
2.60	1.0490D 11	5.4680D 05	1.0490D 06	1.5580D 09	8.8050D 08	1.0000D 06	1.1840D 07	4.5200D-02	1.3700D-03
2.80	1.0180D 11	5.3780D 05	1.0530D 06	1.5800D 09	8.8370D 08	1.0000D 06	1.2410D 07	4.5880D-02	1.3720D-03
3.00	9.8920D 10	5.2860D 05	1.0570D 06	1.5990D 09	8.8690D 08	1.0000D 06	1.2990D 07	4.6520D-02	1.3740D-03
3.20	9.6140D 10	5.1910D 05	1.0610D 06	1.6160D 09	8.9030D 08	1.0000D 06	1.3570D 07	4.7110D-02	1.3770D-03
3.40	9.3510D 10	5.0950D 05	1.0650D 06	1.6310D 09	8.9370D 08	1.0000D 06	1.4160D 07	4.7650D-02	1.3800D-03
3.60	9.1010D 10	4.9990D 05	1.0690D 06	1.6440D 09	8.9720D 08	1.0000D 06	1.4750D 07	4.8150D-02	1.3830D-03
3.80	8.8630D 10	4.9020D 05	1.0730D 06	1.6560D 09	9.0080D 08	1.0000D 06	1.5340D 07	4.8600D-02	1.3860D-03
4.00	8.6370D 10	4.8050D 05	1.0770D 06	1.6660D 09	9.0440D 08	1.0000D 06	1.5940D 07	4.9000D-02	1.3890D-03
4.20	8.4210D 10	4.7080D 05	1.0800D 06	1.6740D 09	9.0800D 08	1.0000D 06	1.6540D 07	4.9360D-02	1.3930D-03
4.40	8.2150D 10	4.6120D 05	1.0840D 06	1.6810D 09	9.1170D 08	1.0000D 06	1.7140D 07	4.9670D-02	1.3960D-03
4.60	8.0180D 10	4.5160D 05	1.0880D 06	1.6860D 09	9.1540D 08	1.0000D 06	1.7730D 07	4.9950D-02	1.3990D-03
4.80	7.8300D 10	4.4220D 05	1.0910D 06	1.6910D 09	9.1920D 08	1.0000D 06	1.8330D 07	5.0180D-02	1.4020D-03
5.00	7.6500D 10	4.3290D 05	1.0950D 06	1.6940D 09	9.2290D 08	1.0000D 06	1.8930D 07	5.0390D-02	1.4050D-03
5.20	7.4770D 10	4.2370D 05	1.0980D 06	1.6960D 09	9.2670D 08	1.0000D 06	1.9530D 07	5.0550D-02	1.4080D-03
5.40	7.3120D 10	4.1470D 05	1.1020D 06	1.6980D 09	9.3040D 08	1.0000D 06	2.0120D 07	5.0690D-02	1.4100D-03
5.60	7.1530D 10	4.0580D 05	1.1050D 06	1.6980D 09	9.3420D 08	1.0000D 06	2.0710D 07	5.0800D-02	1.4130D-03
5.80	7.0010D 10	3.9710D 05	1.1080D 06	1.6970D 09	9.3790D 08	1.0000D 06	2.1310D 07	5.0870D-02	1.4160D-03
6.00	6.8540D 10	3.8850D 05	1.1110D 06	1.6960D 09	9.4170D 08	1.0000D 06	2.1890D 07	5.0930D-02	1.4180D-03
6.20	6.7130D 10	3.8010D 05	1.1140D 06	1.6940D 09	9.4540D 08	1.0000D 06	2.2480D 07	5.0950D-02	1.4210D-03
6.40	6.5780D 10	3.7190D 05	1.1170D 06	1.6910D 09	9.4910D 08	1.0000D 06	2.3060D 07	5.0960D-02	1.4230D-03
6.60	6.4470D 10	3.6390D 05	1.1200D 06	1.6880D 09	9.5280D 08	1.0000D 06	2.3640D 07	5.0940D-02	1.4250D-03
6.80	6.3220D 10	3.5600D 05	1.1230D 06	1.6840D 09	9.5650D 08	1.0000D 06	2.4210D 07	5.0900D-02	1.4280D-03
7.00	6.2000D 10	3.4830D 05	1.1260D 06	1.6800D 09	9.6020D 08	1.0000D 06	2.4780D 07	5.0840D-02	1.4300D-03
7.20	6.0830D 10	3.4080D 05	1.1280D 06	1.6750D 09	9.6380D 08	1.0000D 06	2.5350D 07	5.0770D-02	1.4320D-03
7.40	5.9700D 10	3.3350D 05	1.1310D 06	1.6690D 09	9.6740D 08	1.0000D 06	2.5910D 07	5.0680D-02	1.4340D-03
7.60	5.8610D 10	3.2630D 05	1.1330D 06	1.6630D 09	9.7090D 08	1.0000D 06	2.6460D 07	5.0570D-02	1.4360D-03
7.80	5.7560D 10	3.1940D 05	1.1360D 06	1.6570D 09	9.7450D 08	1.0000D 06	2.7010D 07	5.0450D-02	1.4380D-03
8.00	5.6540D 10	3.1250D 05	1.1380D 06	1.6510D 09	9.7790D 08	1.0000D 06	2.7560D 07	5.0320D-02	1.4400D-03
8.20	5.5550D 10	3.0590D 05	1.1410D 06	1.6440D 09	9.8140D 08	1.0000D 06	2.8100D 07	5.0170D-02	1.4410D-03
8.40	5.4590D 10	2.9940D 05	1.1430D 06	1.6370D 09	9.8480D 08	1.0000D 06	2.8640D 07	5.0020D-02	1.4430D-03
8.60	5.3670D 10	2.9310D 05	1.1450D 06	1.6300D 09	9.8820D 08	1.0000D 06	2.9170D 07	4.9850D-02	1.4450D-03
8.80	5.2770D 10	2.8690D 05	1.1470D 06	1.6220D 09	9.9150D 08	1.0000D 06	2.9690D 07	4.9680D-02	1.4460D-03
9.00	5.1900D 10	2.8090D 05	1.1490D 06	1.6140D 09	9.9480D 08	1.0000D 06	3.0210D 07	4.9490D-02	1.4480D-03
9.20	5.1060D 10	2.7510D 05	1.1510D 06	1.6070D 09	9.9810D 08	1.0000D 06	3.0730D 07	4.9300D-02	1.4490D-03
9.40	5.0240D 10	2.6940D 05	1.1530D 06	1.5980D 09	1.0010D 09	1.0000D 06	3.1230D 07	4.9100D-02	1.4510D-03
9.60	4.9450D 10	2.6390D 05	1.1550D 06	1.5900D 09	1.0040D 09	1.0000D 06	3.1740D 07	4.8900D-02	1.4520D-03
9.80	4.8680D 10	2.5840D 05	1.1570D 06	1.5820D 09	1.0080D 09	1.0000D 06	3.2230D 07	4.8680D-02	1.4540D-03
10.00	4.7930D 10	2.5320D 05	1.1590D 06	1.5730D 09	1.0110D 09	1.0000D 06	3.2730D 07	4.8470D-02	1.4550D-03

T= 800 K, H=15 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.27D 07	1.78D-14
2	2*NO3 >>> 2*NO2 + O2	3.98D-14	5.95D-48
3	NO2 + NO3 >>> NO2 + NO + O2	6.59D-14	3.13D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.74D-18
5	NO + O3 >>> NO2 + O2	3.43D-13	4.42D-26
6	NO2 + O3 >>> NO3 + O2	5.61D-15	9.78D-21
7	HNO3 + M >>> HO + NO2 + M	9.11D 00	2.01D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.43D-18
9	O + O + M >>> O2 + M	3.40D-16	4.32D-15
10	O + O2 + M >>> O3 + M	2.13D-16	1.08D 02
11	O + O3 >>> 2*O2	1.07D-12	6.11D-39
12	O + NO + M >>> NO2 + M	3.41D-14	3.25D-08
13	O + NO2 >>> NO + O2	1.17D-11	5.55D-25
14	O + NO2 + M >>> NO3 + M	1.06D-13	8.48D-24
15	HO + HO >>> H2O + O	5.00D-12	1.06D-15
16	O2 + 2*NO >>> 2*NO2	6.40D-39	8.78D-20
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	9.55D-15
19	O + HO2 >>> HO + O2	4.28D-11	3.43D-24
20	O2 + H + M >>> HO2 + M	1.06D-14	1.58D-03
21	O3 + H >>> HO + O2	5.25D-11	6.31D-34
22	O3 + HO >>> HO2 + O2	4.30D-13	3.24D-24
23	O3 + HO2 >>> HO + 2*O2	1.48D-14	2.35D-48
24	H + HO + M >>> H2O + M	4.13D-14	4.09D-22
25	H + HO2 >>> 2*HO	1.28D-10	2.16D-22
26	H + HO2 >>> H2 + O2	2.71D-11	1.45D-26
27	H + H2O >>> H2 + HO	4.09D-16	1.41D-12
28	H + H2O2 >>> H2 + HO2	3.93D-13	9.47D-18
29	H + H2O2 >>> HO + H2O	5.11D-13	6.02D-33

30	2*HO + M >>> H2O2 + M	4.08D-14	3.37D-02
31	HO + HO2 >>> H2O + O2	4.44D-11	5.70D-30
32	2*HO2 >>> H2O2 + O2	9.10D-12	1.53D-22
33	HO2 + H2O >>> H2O2 + HO	5.19D-20	3.46D-12
34	NO + H + M >>> HNO + M	1.16D-14	6.88D-04
35	NO + HO >>> NO2 + H	3.30D-20	2.30D-10
36	NO + HO + M >>> HNO2 + M	1.64D-13	1.56D 00
37	NO + HO2 >>> NO2 + HO	4.46D-12	7.66D-14
38	H + H + M >>> H2 + M	1.06D-15	1.12D-20
39	HNO4 + M >>> HO2 + NO2 + M	1.33D 07	1.75D-14
40	CLNO3 + M >>> CLO + NO2 + M	1.16D 07	6.67D-15

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	1.000D 07	4.500D 09	2.000D 04	5.000D 09	2.500D 12	8.200D 17	1.500D 09	2.000D 06	7.300D 12
0.20	1.871D-04	1.759D 09	7.621D 07	1.099D 10	1.219D 12	8.200D 17	2.427D 08	3.875D 09	7.299D 12
0.40	1.175D-04	9.157D 08	9.190D 07	1.202D 10	9.991D 11	8.200D 17	3.933D 07	5.223D 09	7.298D 12
0.60	9.895D-05	7.242D 08	9.784D 07	1.224D 10	8.414D 11	8.200D 17	6.441D 06	6.148D 09	7.297D 12
0.80	9.525D-05	6.768D 08	1.008D 08	1.229D 10	7.227D 11	8.200D 17	1.125D 06	6.809D 09	7.297D 12
1.00	9.538D-05	6.674D 08	1.023D 08	1.230D 10	6.304D 11	8.200D 17	2.705D 05	7.277D 09	7.296D 12
1.20	9.630D-05	6.694D 08	1.030D 08	1.230D 10	5.566D 11	8.200D 17	1.367D 05	7.597D 09	7.296D 12
1.40	9.715D-05	6.749D 08	1.031D 08	1.229D 10	4.964D 11	8.200D 17	1.187D 05	7.802D 09	7.296D 12
1.60	9.773D-05	6.816D 08	1.027D 08	1.228D 10	4.465D 11	8.200D 17	1.186D 05	7.920D 09	7.296D 12
1.80	9.799D-05	6.886D 08	1.019D 08	1.228D 10	4.046D 11	8.200D 17	1.205D 05	7.970D 09	7.296D 12
2.00	9.795D-05	6.957D 08	1.008D 08	1.227D 10	3.689D 11	8.200D 17	1.221D 05	7.969D 09	7.296D 12
2.20	9.766D-05	7.026D 08	9.953D 07	1.226D 10	3.382D 11	8.200D 17	1.230D 05	7.930D 09	7.296D 12
2.40	9.713D-05	7.094D 08	9.804D 07	1.226D 10	3.116D 11	8.200D 17	1.234D 05	7.863D 09	7.296D 12
2.60	9.640D-05	7.160D 08	9.641D 07	1.225D 10	2.884D 11	8.200D 17	1.234D 05	7.774D 09	7.296D 12
2.80	9.549D-05	7.224D 08	9.466D 07	1.225D 10	2.679D 11	8.200D 17	1.230D 05	7.670D 09	7.296D 12
3.00	9.445D-05	7.286D 08	9.283D 07	1.224D 10	2.498D 11	8.200D 17	1.223D 05	7.556D 09	7.296D 12
3.20	9.328D-05	7.346D 08	9.093D 07	1.224D 10	2.336D 11	8.200D 17	1.214D 05	7.435D 09	7.296D 12
3.40	9.200D-05	7.403D 08	8.899D 07	1.224D 10	2.192D 11	8.200D 17	1.204D 05	7.310D 09	7.296D 12
3.60	9.064D-05	7.459D 08	8.701D 07	1.223D 10	2.062D 11	8.200D 17	1.193D 05	7.182D 09	7.296D 12
3.80	8.920D-05	7.513D 08	8.502D 07	1.223D 10	1.944D 11	8.200D 17	1.180D 05	7.054D 09	7.296D 12
4.00	8.771D-05	7.566D 08	8.302D 07	1.223D 10	1.837D 11	8.200D 17	1.167D 05	6.926D 09	7.296D 12
4.20	8.617D-05	7.616D 08	8.102D 07	1.222D 10	1.740D 11	8.200D 17	1.154D 05	6.800D 09	7.296D 12
4.40	8.459D-05	7.666D 08	7.902D 07	1.222D 10	1.652D 11	8.200D 17	1.140D 05	6.676D 09	7.296D 12
4.60	8.298D-05	7.713D 08	7.704D 07	1.222D 10	1.570D 11	8.200D 17	1.127D 05	6.554D 09	7.297D 12
4.80	8.136D-05	7.759D 08	7.509D 07	1.222D 10	1.496D 11	8.200D 17	1.113D 05	6.435D 09	7.297D 12
5.00	7.972D-05	7.804D 08	7.315D 07	1.221D 10	1.427D 11	8.200D 17	1.099D 05	6.319D 09	7.297D 12
5.20	7.808D-05	7.848D 08	7.124D 07	1.221D 10	1.363D 11	8.200D 17	1.086D 05	6.207D 09	7.297D 12
5.40	7.643D-05	7.890D 08	6.937D 07	1.221D 10	1.304D 11	8.200D 17	1.072D 05	6.097D 09	7.297D 12
5.60	7.479D-05	7.931D 08	6.753D 07	1.221D 10	1.249D 11	8.200D 17	1.059D 05	5.991D 09	7.297D 12
5.80	7.316D-05	7.971D 08	6.572D 07	1.221D 10	1.198D 11	8.200D 17	1.046D 05	5.888D 09	7.297D 12
6.00	7.154D-05	8.010D 08	6.395D 07	1.220D 10	1.151D 11	8.200D 17	1.033D 05	5.789D 09	7.297D 12
6.20	6.993D-05	8.048D 08	6.222D 07	1.220D 10	1.106D 11	8.200D 17	1.021D 05	5.693D 09	7.297D 12
6.40	6.834D-05	8.085D 08	6.053D 07	1.220D 10	1.064D 11	8.200D 17	1.009D 05	5.600D 09	7.297D 12
6.60	6.677D-05	8.122D 08	5.887D 07	1.220D 10	1.025D 11	8.200D 17	9.968D 04	5.510D 09	7.297D 12
6.80	6.522D-05	8.157D 08	5.726D 07	1.220D 10	9.884D 10	8.200D 17	9.853D 04	5.423D 09	7.297D 12
7.00	6.370D-05	8.191D 08	5.569D 07	1.219D 10	9.539D 10	8.200D 17	9.740D 04	5.338D 09	7.297D 12
7.20	6.220D-05	8.225D 08	5.416D 07	1.219D 10	9.213D 10	8.200D 17	9.629D 04	5.257D 09	7.298D 12
7.40	6.073D-05	8.258D 08	5.266D 07	1.219D 10	8.905D 10	8.200D 17	9.522D 04	5.178D 09	7.298D 12
7.60	5.928D-05	8.290D 08	5.121D 07	1.219D 10	8.614D 10	8.200D 17	9.418D 04	5.102D 09	7.298D 12
7.80	5.787D-05	8.322D 08	4.980D 07	1.219D 10	8.339D 10	8.200D 17	9.316D 04	5.028D 09	7.298D 12
8.00	5.648D-05	8.353D 08	4.842D 07	1.219D 10	8.078D 10	8.200D 17	9.217D 04	4.957D 09	7.298D 12
8.20	5.512D-05	8.383D 08	4.709D 07	1.218D 10	7.830D 10	8.200D 17	9.120D 04	4.888D 09	7.298D 12
8.40	5.379D-05	8.413D 08	4.579D 07	1.218D 10	7.595D 10	8.200D 17	9.026D 04	4.821D 09	7.298D 12
8.60	5.249D-05	8.442D 08	4.453D 07	1.218D 10	7.372D 10	8.200D 17	8.935D 04	4.756D 09	7.298D 12
8.80	5.122D-05	8.470D 08	4.330D 07	1.218D 10	7.159D 10	8.200D 17	8.846D 04	4.694D 09	7.298D 12
9.00	4.998D-05	8.498D 08	4.211D 07	1.218D 10	6.956D 10	8.200D 17	8.759D 04	4.633D 09	7.298D 12
9.20	4.877D-05	8.526D 08	4.096D 07	1.218D 10	6.762D 10	8.200D 17	8.675D 04	4.574D 09	7.298D 12
9.40	4.759D-05	8.553D 08	3.984D 07	1.217D 10	6.578D 10	8.200D 17	8.593D 04	4.517D 09	7.298D 12
9.60	4.643D-05	8.580D 08	3.875D 07	1.217D 10	6.401D 10	8.200D 17	8.513D 04	4.461D 09	7.298D 12
9.80	4.531D-05	8.606D 08	3.770D 07	1.217D 10	6.233D 10	8.200D 17	8.435D 04	4.407D 09	7.298D 12
10.00	4.421D-05	8.632D 08	3.668D 07	1.217D 10	6.071D 10	8.200D 17	8.359D 04	4.355D 09	7.298D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000 06	1.0000 06	1.0000 06	1.5000 07	8.5000 08	1.0000 06	6.0000 06	2.0000 09	5.0000 07
0.20	7.566D 11	7.437D 06	1.048D 06	1.893D 09	8.467D 08	1.000D 06	5.129D 06	4.357D-03	7.052D-05
0.40	6.202D 11	8.225D 06	1.150D 06	2.625D 09	8.480D 08	1.000D 06	5.278D 06	3.146D-03	3.672D-05
0.60	5.223D 11	8.157D 06	1.283D 06	3.115D 09	8.544D 08	1.000D 06	5.827D 06	2.952D-03	2.904D-05
0.80	4.487D 11	7.764D 06	1.428D 06	3.461D 09	8.648D 08	1.000D 06	6.515D 06	3.066D-03	2.714D-05
1.00	3.914D 11	7.240D 06	1.576D 06	3.703D 09	8.786D 08	1.000D 06	7.215D 06	3.235D-03	2.677D-05
1.20	3.456D 11	6.676D 06	1.720D 06	3.867D 09	8.946D 08	1.000D 06	7.861D 06	3.388D-03	2.684D-05
1.40	3.082D 11	6.117D 06	1.857D 06	3.970D 09	9.122D 08	1.000D 06	8.422D 06	3.507D-03	2.706D-05
1.60	2.773D 11	5.586D 06	1.983D 06	4.027D 09	9.306D 08	1.000D 06	8.885D 06	3.592D-03	2.733D-05
1.80	2.512D 11	5.094D 06	2.099D 06	4.048D 09	9.493D 08	1.000D 06	9.250D 06	3.648D-03	2.762D-05
2.00	2.291D 11	4.645D 06	2.204D 06	4.043D 09	9.679D 08	1.000D 06	9.523D 06	3.681D-03	2.790D-05
2.20	2.100D 11	4.239D 06	2.299D 06	4.017D 09	9.860D 08	1.000D 06	9.715D 06	3.694D-03	2.818D-05
2.40	1.935D 11	3.872D 06	2.385D 06	3.977D 09	1.003D 09	1.000D 06	9.834D 06	3.693D-03	2.845D-05
2.60	1.791D 11	3.543D 06	2.461D 06	3.926D 09	1.020D 09	1.000D 06	9.893D 06	3.679D-03	2.871D-05
2.80	1.664D 11	3.249D 06	2.530D 06	3.867D 09	1.036D 09	1.000D 06	9.902D 06	3.656D-03	2.897D-05
3.00	1.551D 11	2.984D 06	2.591D 06	3.803D 09	1.050D 09	1.000D 06	9.870D 06	3.627D-03	2.922D-05
3.20	1.451D 11	2.747D 06	2.646D 06	3.736D 09	1.064D 09	1.000D 06	9.805D 06	3.592D-03	2.946D-05
3.40	1.361D 11	2.534D 06	2.695D 06	3.666D 09	1.077D 09	1.000D 06	9.713D 06	3.552D-03	2.969D-05
3.60	1.281D 11	2.342D 06	2.739D 06	3.596D 09	1.088D 09	1.000D 06	9.602D 06	3.510D-03	2.991D-05
3.80	1.208D 11	2.169D 06	2.779D 06	3.525D 09	1.099D 09	1.000D 06	9.476D 06	3.466D-03	3.013D-05
4.00	1.142D 11	2.013D 06	2.814D 06	3.455D 09	1.109D 09	1.000D 06	9.339D 06	3.421D-03	3.034D-05
4.20	1.081D 11	1.872D 06	2.846D 06	3.386D 09	1.118D 09	9.999D 05	9.195D 06	3.375D-03	3.054D-05
4.40	1.026D 11	1.744D 06	2.875D 06	3.318D 09	1.126D 09	9.998D 05	9.045D 06	3.328D-03	3.074D-05
4.60	9.758D 10	1.628D 06	2.901D 06	3.251D 09	1.133D 09	9.997D 05	8.893D 06	3.282D-03	3.093D-05
4.80	9.294D 10	1.523D 06	2.924D 06	3.186D 09	1.139D 09	9.996D 05	8.740D 06	3.236D-03	3.112D-05
5.00	8.866D 10	1.427D 06	2.945D 06	3.123D 09	1.145D 09	9.995D 05	8.587D 06	3.190D-03	3.130D-05
5.20	8.470D 10	1.339D 06	2.964D 06	3.061D 09	1.150D 09	9.994D 05	8.436D 06	3.144D-03	3.147D-05
5.40	8.103D 10	1.258D 06	2.981D 06	3.002D 09	1.154D 09	9.993D 05	8.286D 06	3.100D-03	3.164D-05
5.60	7.763D 10	1.184D 06	2.996D 06	2.944D 09	1.158D 09	9.992D 05	8.139D 06	3.056D-03	3.181D-05
5.80	7.446D 10	1.117D 06	3.010D 06	2.888D 09	1.161D 09	9.991D 05	7.996D 06	3.013D-03	3.197D-05
6.00	7.150D 10	1.054D 06	3.023D 06	2.834D 09	1.164D 09	9.990D 05	7.856D 06	2.971D-03	3.212D-05
6.20	6.873D 10	9.966D 05	3.034D 06	2.781D 09	1.166D 09	9.989D 05	7.719D 06	2.930D-03	3.228D-05
6.40	6.614D 10	9.434D 05	3.045D 06	2.730D 09	1.168D 09	9.988D 05	7.587D 06	2.889D-03	3.243D-05
6.60	6.372D 10	8.941D 05	3.054D 06	2.681D 09	1.169D 09	9.987D 05	7.458D 06	2.850D-03	3.257D-05
6.80	6.143D 10	8.485D 05	3.062D 06	2.634D 09	1.170D 09	9.986D 05	7.333D 06	2.812D-03	3.271D-05
7.00	5.928D 10	8.061D 05	3.070D 06	2.588D 09	1.170D 09	9.985D 05	7.212D 06	2.774D-03	3.285D-05
7.20	5.726D 10	7.667D 05	3.077D 06	2.544D 09	1.170D 09	9.983D 05	7.095D 06	2.738D-03	3.298D-05
7.40	5.535D 10	7.300D 05	3.083D 06	2.501D 09	1.170D 09	9.982D 05	6.982D 06	2.703D-03	3.312D-05
7.60	5.354D 10	6.958D 05	3.089D 06	2.459D 09	1.169D 09	9.981D 05	6.872D 06	2.668D-03	3.325D-05
7.80	5.183D 10	6.639D 05	3.094D 06	2.419D 09	1.168D 09	9.980D 05	6.766D 06	2.634D-03	3.337D-05
8.00	5.021D 10	6.340D 05	3.098D 06	2.380D 09	1.167D 09	9.979D 05	6.663D 06	2.602D-03	3.350D-05
8.20	4.867D 10	6.060D 05	3.102D 06	2.342D 09	1.165D 09	9.977D 05	6.563D 06	2.570D-03	3.362D-05
8.40	4.721D 10	5.798D 05	3.106D 06	2.306D 09	1.164D 09	9.976D 05	6.467D 06	2.538D-03	3.374D-05
8.60	4.582D 10	5.552D 05	3.109D 06	2.270D 09	1.162D 09	9.975D 05	6.374D 06	2.508D-03	3.385D-05
8.80	4.450D 10	5.321D 05	3.112D 06	2.236D 09	1.159D 09	9.974D 05	6.283D 06	2.479D-03	3.397D-05
9.00	4.324D 10	5.103D 05	3.114D 06	2.203D 09	1.157D 09	9.973D 05	6.196D 06	2.450D-03	3.408D-05
9.20	4.204D 10	4.898D 05	3.117D 06	2.170D 09	1.154D 09	9.971D 05	6.111D 06	2.422D-03	3.419D-05
9.40	4.089D 10	4.705D 05	3.119D 06	2.139D 09	1.152D 09	9.970D 05	6.029D 06	2.394D-03	3.430D-05
9.60	3.979D 10	4.523D 05	3.120D 06	2.108D 09	1.149D 09	9.969D 05	5.950D 06	2.367D-03	3.441D-05
9.80	3.874D 10	4.350D 05	3.122D 06	2.079D 09	1.145D 09	9.968D 05	5.872D 06	2.341D-03	3.451D-05
10.00	3.774D 10	4.187D 05	3.123D 06	2.050D 09	1.142D 09	9.966D 05	5.798D 06	2.316D-03	3.462D-05

T= 250 K, H= 20 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N205 + M >>> NO2 +NO3 + M	8.90D-06	2.78D-13
2	2*NO3 >>> 2*NO2 + O2	4.71D-17	7.46D-62
3	NO2 + NO3 >>> NO2 + NO + O2	4.21D-15	1.19D-34
4	NO3 + NO >>> 2*NO2	1.90D-11	3.29D-32
5	NO + O3 >>> NO2 + O2	6.36D-15	1.08D-56
6	NO2 + O3 >>> NO3 + O2	6.65D-18	8.33D-39
7	HNO3 + M >>> HO + NO2 + M	1.18D-27	5.41D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.80D-29
9	O + O + M >>> O2 + M	5.92D-15	6.95D-57
10	O + O2 + M >>> O3 + M	1.27D-15	3.55D-12
11	O + O3 >>> 2*O2	1.92D-15	0.0
12	O + NO + M >>> NO2 + M	2.49D-13	1.85D-47
13	O + NO2 >>> NO + O2	5.12D-12	6.27D-53
14	O + NO2 + M >>> NO3 + M	1.56D-13	1.24D-23
15	HO + HO >>> H2O + O	1.09D-12	9.77D-27
16	O2 + 2*NO >>> 2*NO2	2.75D-38	3.88D-35
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	7.73D-25
19	O + HO2 >>> HO + O2	1.08D-11	5.45D-60
20	O2 + H + M >>> HO2 + M	6.13D-14	7.85D-31
21	O3 + H >>> HO + O2	1.27D-11	0.0
22	O3 + HO >>> HO2 + O2	2.75D-14	1.04D-48
23	O3 + HO2 >>> HO + 2*O2	4.45D-16	2.41D-68
24	H + HO + M >>> H2O + M	1.25D-12	0.0
25	H + HO2 >>> 2*HO	9.40D-12	1.62D-46
26	H + HO2 >>> H2 + O2	1.04D-11	2.55D-61
27	H + H2O >>> H2 + HO	2.34D-28	1.14D-15
28	H + H2O2 >>> H2 + HO2	8.36D-15	5.62D-29
29	H + H2O2 >>> HO + H2O	1.09D-14	1.35D-75

30	2*HO + M >>> H2O2 + M	7.11D-13	1.91D-31
31	HO + HO2 >>> H2O + O2	1.12D-11	3.89D-74
32	2*HO2 >>> H2O2 + O2	2.30D-12	8.58D-49
33	HO2 + H2O >>> H2O2 + HO	1.02D-39	5.49D-13
34	NO + H + M >>> HNO + M	3.87D-14	6.06D-33
35	NO + HO >>> NO2 + H	3.05D-38	3.01D-11
36	NO + HO + M >>> HNO2 + M	5.09D-12	1.93D-28
37	NO + HO2 >>> NO2 + HO	1.65D-13	7.47D-21
38	H + H + M >>> H2 + M	1.56D-15	0.0
39	HNO4 + M >>> HO2 + NO2 + M	2.06D-05	3.79D-13
40	CLNO3 + M >>> CLO + NO2 + M	7.18D-07	3.18D-13

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.0000D 08	8.0000D 09	5.0000D 05	1.5000D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.0000D 06	3.8000D 12
0.20	4.0000D 08	8.0080D 09	5.4560D 05	1.4910D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.7710D 05	3.8000D 12
0.40	4.0000D 08	8.0170D 09	5.9100D 05	1.4830D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.5260D 05	3.8000D 12
0.60	4.0000D 08	8.0250D 09	6.3620D 05	1.4740D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.2900D 05	3.8000D 12
0.80	4.0000D 08	8.0340D 09	6.8120D 05	1.4660D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.0620D 05	3.8000D 12
1.00	4.0000D 08	8.0420D 09	7.2600D 05	1.4580D 09	4.5000D 12	3.8000D 17	4.0000D 09	8.8420D 05	3.8000D 12
1.20	4.0000D 08	8.0500D 09	7.7060D 05	1.4490D 09	4.5000D 12	3.8000D 17	4.0000D 09	8.6290D 05	3.8000D 12
1.40	4.0000D 08	8.0580D 09	8.1500D 05	1.4410D 09	4.5000D 12	3.8000D 17	4.0000D 09	8.4240D 05	3.8000D 12
1.60	4.0000D 08	8.0670D 09	8.5920D 05	1.4330D 09	4.5000D 12	3.8000D 17	4.0000D 09	8.2260D 05	3.8000D 12
1.80	4.0000D 08	8.0750D 09	9.0320D 05	1.4250D 09	4.5000D 12	3.8000D 17	4.0000D 09	8.0340D 05	3.8000D 12
2.00	4.0000D 08	8.0830D 09	9.4700D 05	1.4170D 09	4.5000D 12	3.8000D 17	4.0000D 09	7.8500D 05	3.8000D 12
2.20	4.0000D 08	8.0910D 09	9.9070D 05	1.4080D 09	4.5000D 12	3.8000D 17	4.0000D 09	7.6710D 05	3.8000D 12
2.40	4.0000D 08	8.0990D 09	1.0340D 06	1.4000D 09	4.5000D 12	3.8000D 17	4.0000D 09	7.4990D 05	3.8000D 12
2.60	4.0000D 08	8.1070D 09	1.0770D 06	1.3920D 09	4.5000D 12	3.8000D 17	4.0000D 09	7.3330D 05	3.8000D 12
2.80	4.0000D 08	8.1150D 09	1.1210D 06	1.3840D 09	4.5000D 12	3.8000D 17	4.0000D 09	7.1720D 05	3.8000D 12
3.00	4.0000D 08	8.1220D 09	1.1640D 06	1.3770D 09	4.5000D 12	3.8000D 17	4.0000D 09	7.0170D 05	3.8000D 12
3.20	4.0000D 08	8.1300D 09	1.2060D 06	1.3690D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.8680D 05	3.8000D 12
3.40	4.0000D 08	8.1380D 09	1.2490D 06	1.3610D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.7230D 05	3.8000D 12
3.60	4.0000D 08	8.1460D 09	1.2910D 06	1.3530D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.5840D 05	3.8000D 12
3.80	4.0000D 08	8.1530D 09	1.3340D 06	1.3450D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.4490D 05	3.8000D 12
4.00	4.0000D 08	8.1610D 09	1.3760D 06	1.3380D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.3190D 05	3.8000D 12
4.20	4.0000D 08	8.1690D 09	1.4180D 06	1.3300D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.1940D 05	3.8000D 12
4.40	4.0000D 08	8.1760D 09	1.4600D 06	1.3220D 09	4.5000D 12	3.8000D 17	4.0000D 09	6.0730D 05	3.8000D 12
4.60	4.0000D 08	8.1840D 09	1.5020D 06	1.3150D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.9560D 05	3.8000D 12
4.80	4.0000D 08	8.1910D 09	1.5430D 06	1.3070D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.8430D 05	3.8000D 12
5.00	4.0000D 08	8.1980D 09	1.5850D 06	1.3000D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.7330D 05	3.8000D 12
5.20	4.0000D 08	8.2060D 09	1.6260D 06	1.2920D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.6280D 05	3.8000D 12
5.40	4.0000D 08	8.2130D 09	1.6670D 06	1.2850D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.5260D 05	3.8000D 12
5.60	4.0000D 08	8.2200D 09	1.7080D 06	1.2780D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.4280D 05	3.8000D 12
5.80	4.0000D 08	8.2280D 09	1.7490D 06	1.2700D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.3330D 05	3.8000D 12
6.00	4.0000D 08	8.2350D 09	1.7900D 06	1.2630D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.2420D 05	3.8000D 12
6.20	4.0000D 08	8.2420D 09	1.8310D 06	1.2560D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.1530D 05	3.8000D 12
6.40	4.0000D 08	8.2490D 09	1.8710D 06	1.2490D 09	4.5000D 12	3.8000D 17	4.0000D 09	5.0680D 05	3.8000D 12
6.60	4.0000D 08	8.2560D 09	1.9110D 06	1.2420D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.9850D 05	3.8000D 12
6.80	4.0000D 08	8.2630D 09	1.9520D 06	1.2350D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.9050D 05	3.8000D 12
7.00	4.0000D 08	8.2700D 09	1.9920D 06	1.2270D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.8280D 05	3.8000D 12
7.20	4.0000D 08	8.2770D 09	2.0320D 06	1.2200D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.7540D 05	3.8000D 12
7.40	4.0000D 08	8.2840D 09	2.0720D 06	1.2140D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.6820D 05	3.8000D 12
7.60	4.0000D 08	8.2910D 09	2.1120D 06	1.2070D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.6130D 05	3.8000D 12
7.80	4.0000D 08	8.2980D 09	2.1520D 06	1.2000D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.5460D 05	3.8000D 12
8.00	4.0000D 08	8.3050D 09	2.1910D 06	1.1930D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.4810D 05	3.8000D 12
8.20	4.0000D 08	8.3110D 09	2.2310D 06	1.1860D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.4190D 05	3.8000D 12
8.40	4.0000D 08	8.3180D 09	2.2700D 06	1.1790D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.3580D 05	3.8000D 12
8.60	4.0000D 08	8.3250D 09	2.3100D 06	1.1720D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.3000D 05	3.8000D 12
8.80	4.0000D 08	8.3310D 09	2.3490D 06	1.1660D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.2440D 05	3.8000D 12
9.00	4.0000D 08	8.3380D 09	2.3880D 06	1.1590D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.1890D 05	3.8000D 12
9.20	4.0000D 08	8.3450D 09	2.4270D 06	1.1530D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.1370D 05	3.8000D 12
9.40	4.0000D 08	8.3510D 09	2.4660D 06	1.1460D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.0860D 05	3.8000D 12
9.60	4.0000D 08	8.3580D 09	2.5050D 06	1.1390D 09	4.5000D 12	3.8000D 17	4.0000D 09	4.0370D 05	3.8000D 12
9.80	4.0000D 08	8.3640D 09	2.5440D 06	1.1330D 09	4.5000D 12	3.8000D 17	4.0000D 09	3.9900D 05	3.8000D 12
10.00	4.0000D 08	8.3700D 09	2.5830D 06	1.1260D 09	4.5000D 12	3.8000D 17	4.0000D 09	3.9440D 05	3.8000D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.000D 06	1.000D 06	1.000D 06	2.000D 07	1.300D 09	1.000D 06	1.000D 06	4.000D 09	1.000D 08
0.20	3.534D-02	4.780D-08	1.000D 06	2.102D 07	1.300D 09	1.000D 06	1.002D 06	4.000D 09	1.000D 08
0.40	3.524D-02	4.661D-08	1.000D 06	2.103D 07	1.300D 09	1.000D 06	1.003D 06	4.000D 09	1.000D 08
0.60	3.514D-02	4.545D-08	1.000D 06	2.105D 07	1.300D 09	1.000D 06	1.004D 06	4.000D 09	1.001D 08
0.80	3.504D-02	4.433D-08	1.000D 06	2.107D 07	1.300D 09	1.000D 06	1.006D 06	4.000D 09	1.001D 08
1.00	3.495D-02	4.326D-08	1.000D 06	2.108D 07	1.300D 09	1.000D 06	1.007D 06	4.000D 09	1.001D 08
1.20	3.487D-02	4.222D-08	1.000D 06	2.110D 07	1.300D 09	1.000D 06	1.008D 06	4.000D 09	1.001D 08
1.40	3.479D-02	4.121D-08	1.000D 06	2.111D 07	1.300D 09	1.000D 06	1.010D 06	4.000D 09	1.001D 08
1.60	3.472D-02	4.024D-08	1.000D 06	2.113D 07	1.300D 09	1.000D 06	1.011D 06	4.000D 09	1.001D 08
1.80	3.465D-02	3.931D-08	1.000D 06	2.114D 07	1.300D 09	1.000D 06	1.012D 06	4.000D 09	1.002D 08
2.00	3.458D-02	3.840D-08	1.000D 06	2.115D 07	1.300D 09	1.000D 06	1.013D 06	4.000D 09	1.002D 08
2.20	3.452D-02	3.753D-08	1.000D 06	2.117D 07	1.300D 09	1.000D 06	1.014D 06	4.000D 09	1.002D 08
2.40	3.446D-02	3.669D-08	1.000D 06	2.118D 07	1.300D 09	1.000D 06	1.015D 06	4.000D 09	1.002D 08
2.60	3.440D-02	3.587D-08	1.000D 06	2.119D 07	1.300D 09	1.000D 06	1.016D 06	4.000D 09	1.002D 08
2.80	3.435D-02	3.509D-08	1.000D 06	2.120D 07	1.300D 09	1.000D 06	1.017D 06	4.000D 09	1.002D 08
3.00	3.430D-02	3.433D-08	1.000D 06	2.121D 07	1.300D 09	1.000D 06	1.018D 06	4.000D 09	1.003D 08
3.20	3.425D-02	3.360D-08	1.000D 06	2.123D 07	1.300D 09	1.000D 06	1.019D 06	4.000D 09	1.003D 08
3.40	3.421D-02	3.289D-08	1.000D 06	2.124D 07	1.300D 09	1.000D 06	1.020D 06	4.000D 09	1.003D 08
3.60	3.417D-02	3.221D-08	1.000D 06	2.125D 07	1.300D 09	1.000D 06	1.021D 06	4.000D 09	1.003D 08
3.80	3.413D-02	3.155D-08	1.000D 06	2.126D 07	1.300D 09	1.000D 06	1.022D 06	4.000D 09	1.003D 08
4.00	3.409D-02	3.092D-08	1.000D 06	2.126D 07	1.300D 09	1.000D 06	1.023D 06	4.000D 09	1.004D 08
4.20	3.405D-02	3.030D-08	1.000D 06	2.127D 07	1.300D 09	1.000D 06	1.024D 06	4.000D 09	1.004D 08
4.40	3.402D-02	2.971D-08	1.000D 06	2.128D 07	1.300D 09	1.000D 06	1.025D 06	4.000D 09	1.004D 08
4.60	3.399D-02	2.914D-08	1.000D 06	2.129D 07	1.300D 09	1.000D 06	1.026D 06	4.000D 09	1.004D 08
4.80	3.396D-02	2.858D-08	1.000D 06	2.130D 07	1.300D 09	1.000D 06	1.026D 06	4.000D 09	1.004D 08
5.00	3.393D-02	2.805D-08	1.000D 06	2.131D 07	1.300D 09	1.000D 06	1.027D 06	4.000D 09	1.004D 08
5.20	3.390D-02	2.753D-08	1.000D 06	2.131D 07	1.300D 09	1.000D 06	1.028D 06	4.000D 09	1.005D 08
5.40	3.388D-02	2.704D-08	1.000D 06	2.132D 07	1.300D 09	1.000D 06	1.029D 06	4.000D 09	1.005D 08
5.60	3.385D-02	2.656D-08	1.000D 06	2.133D 07	1.300D 09	1.000D 06	1.029D 06	4.000D 09	1.005D 08
5.80	3.383D-02	2.609D-08	1.000D 06	2.133D 07	1.300D 09	1.000D 06	1.030D 06	4.000D 09	1.005D 08
6.00	3.381D-02	2.564D-08	1.000D 06	2.134D 07	1.300D 09	1.000D 06	1.031D 06	4.000D 09	1.005D 08
6.20	3.379D-02	2.521D-08	1.000D 06	2.135D 07	1.300D 09	1.000D 06	1.031D 06	4.000D 09	1.006D 08
6.40	3.377D-02	2.479D-08	1.000D 06	2.135D 07	1.300D 09	1.000D 06	1.032D 06	4.000D 09	1.006D 08
6.60	3.375D-02	2.439D-08	1.000D 06	2.136D 07	1.300D 09	1.000D 06	1.033D 06	4.000D 09	1.006D 08
6.80	3.373D-02	2.400D-08	1.000D 06	2.136D 07	1.300D 09	1.000D 06	1.033D 06	4.000D 09	1.006D 08
7.00	3.371D-02	2.362D-08	1.000D 06	2.137D 07	1.300D 09	1.000D 06	1.034D 06	4.000D 09	1.006D 08
7.20	3.370D-02	2.326D-08	1.000D 06	2.137D 07	1.300D 09	1.000D 06	1.034D 06	4.000D 09	1.006D 08
7.40	3.368D-02	2.291D-08	1.000D 06	2.138D 07	1.300D 09	1.000D 06	1.035D 06	4.000D 09	1.007D 08
7.60	3.367D-02	2.257D-08	1.000D 06	2.138D 07	1.300D 09	1.000D 06	1.036D 06	4.000D 09	1.007D 08
7.80	3.365D-02	2.224D-08	1.000D 06	2.139D 07	1.300D 09	1.000D 06	1.036D 06	4.000D 09	1.007D 08
8.00	3.364D-02	2.192D-08	1.000D 06	2.139D 07	1.300D 09	1.000D 06	1.037D 06	4.000D 09	1.007D 08
8.20	3.363D-02	2.162D-08	1.000D 06	2.140D 07	1.300D 09	1.000D 06	1.037D 06	4.000D 09	1.007D 08
8.40	3.362D-02	2.132D-08	1.000D 06	2.140D 07	1.300D 09	1.000D 06	1.038D 06	4.000D 09	1.008D 08
8.60	3.360D-02	2.104D-08	1.000D 06	2.140D 07	1.300D 09	1.000D 06	1.038D 06	4.000D 09	1.008D 08
8.80	3.359D-02	2.076D-08	1.000D 06	2.141D 07	1.300D 09	1.000D 06	1.039D 06	4.000D 09	1.008D 08
9.00	3.358D-02	2.050D-08	1.000D 06	2.141D 07	1.300D 09	1.000D 06	1.039D 06	4.000D 09	1.008D 08
9.20	3.357D-02	2.024D-08	1.000D 06	2.142D 07	1.300D 09	1.000D 06	1.040D 06	4.000D 09	1.008D 08
9.40	3.356D-02	1.999D-08	1.000D 06	2.142D 07	1.300D 09	1.000D 06	1.040D 06	4.000D 09	1.008D 08
9.60	3.356D-02	1.975D-08	1.000D 06	2.142D 07	1.300D 09	1.000D 06	1.041D 06	4.000D 09	1.009D 08
9.80	3.355D-02	1.952D-08	1.000D 06	2.142D 07	1.300D 09	1.000D 06	1.041D 06	4.000D 09	1.009D 08
10.00	3.354D-02	1.929D-08	1.000D 06	2.143D 07	1.300D 09	1.000D 06	1.042D 06	4.000D 09	1.009D 08

T=300 K, H= 20 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	7.20D-03	1.31D-13
2	2*NO3 >>> 2*NO2 + O2	2.41D-16	1.75D-58
3	NO2 + NO3 >>> NO2 + NO + O2	8.21D-15	4.92D-35
4	NO3 + NO >>> 2*NO2	1.90D-11	6.98D-29
5	NO + O3 >>> NO2 + O2	1.67D-14	2.85D-49
6	NO2 + O3 >>> NO3 + O2	3.41D-17	2.00D-34
7	HNO3 + M >>> HO + NO2 + M	8.82D-21	2.86D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	1.25D-26
9	O + O + M >>> O2 + M	2.71D-15	2.65D-57
10	O + O2 + M >>> O3 + M	7.52D-16	6.04D-09
11	O + O3 >>> 2*O2	8.90D-15	0.0
12	O + NO + M >>> NO2 + M	1.41D-13	5.52D-38
13	O + NO2 >>> NO + O2	6.25D-12	3.73D-46
14	O + NO2 + M >>> NO3 + M	1.30D-13	1.04D-23
15	HO + HO >>> H2O + O	1.57D-12	4.63D-24
16	O2 + 2*NO >>> 2*NO2	1.93D-38	2.26D-31
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.16D-22
19	O + HO2 >>> HO + O2	1.51D-11	8.51D-52
20	O2 + H + M >>> HO2 + M	3.66D-14	2.98D-24
21	O3 + H >>> HO + O2	1.79D-11	1.62D-69
22	O3 + HO >>> HO2 + O2	5.35D-14	8.98D-43
23	O3 + HO2 >>> HO + 2*O2	1.04D-15	1.53D-63
24	H + HO + M >>> H2O + M	6.47D-13	5.24D-75
25	H + HO2 >>> 2*HO	1.77D-11	1.14D-40
26	H + HO2 >>> H2 + O2	1.31D-11	6.80D-53
27	H + H2O >>> H2 + HO	2.18D-25	6.41D-15
28	H + H2O2 >>> H2 + HO2	2.13D-14	2.96D-26
29	H + H2O2 >>> HO + H2O	2.76D-14	2.95D-65

30	2*HO + M >>> H2O2 + M	3.25D-13	2.37D-24
31	HO + HO2 >>> H2O + O2	1.57D-11	1.98D-63
32	2*HO2 >>> H2O2 + O2	3.21D-12	1.98D-42
33	HO2 + H2O >>> H2O2 + HO	6.11D-35	8.57D-13
34	NO + H + M >>> HNO + M	2.64D-14	6.77D-26
35	NO + HO >>> NO2 + H	7.19D-34	4.92D-11
36	NO + HO + M >>> HNO2 + M	2.02D-12	1.14D-21
37	NO + HO2 >>> NO2 + HO	3.66D-13	3.74D-19
38	H + H + M >>> H2 + M	1.30D-15	1.12D-68
39	HNO4 + M >>> HO2 + NO2 + M	1.40D-02	1.68D-13
40	CLNO3 + M >>> CLO + NO2 + M	1.05D-03	1.57D-13

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.0000D 08	8.0000D 09	5.0000D 05	1.5000D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.0000D 06	3.8000D 12
0.20	3.9940D 08	8.0340D 09	1.3160D 06	1.4780D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.8030D 05	3.8000D 12
0.40	3.9880D 08	8.0680D 09	2.1280D 06	1.4560D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.6750D 05	3.8000D 12
0.60	3.9830D 08	8.1010D 09	2.9360D 06	1.4340D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.6660D 05	3.8000D 12
0.80	3.9770D 08	8.1340D 09	3.7390D 06	1.4120D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.7680D 05	3.8000D 12
1.00	3.9710D 08	8.1660D 09	4.5390D 06	1.3910D 09	4.5000D 12	3.8000D 17	4.0000D 09	9.9750D 05	3.8000D 12
1.20	3.9660D 08	8.1980D 09	5.3350D 06	1.3700D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.0280D 06	3.8000D 12
1.40	3.9600D 08	8.2300D 09	6.1260D 06	1.3500D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.0680D 06	3.8000D 12
1.60	3.9540D 08	8.2620D 09	6.9150D 06	1.3300D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.1170D 06	3.8000D 12
1.80	3.9490D 08	8.2930D 09	7.6990D 06	1.3100D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.1730D 06	3.8000D 12
2.00	3.9430D 08	8.3240D 09	8.4810D 06	1.2900D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.2380D 06	3.8000D 12
2.20	3.9370D 08	8.3540D 09	9.2590D 06	1.2710D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.3090D 06	3.8000D 12
2.40	3.9320D 08	8.3840D 09	1.0030D 07	1.2520D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.3880D 06	3.8000D 12
2.60	3.9260D 08	8.4140D 09	1.0810D 07	1.2330D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.4720D 06	3.8000D 12
2.80	3.9200D 08	8.4440D 09	1.1570D 07	1.2150D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.5630D 06	3.8000D 12
3.00	3.9150D 08	8.4730D 09	1.2340D 07	1.1960D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.6590D 06	3.8000D 12
3.20	3.9090D 08	8.5020D 09	1.3100D 07	1.1780D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.7600D 06	3.8000D 12
3.40	3.9040D 08	8.5310D 09	1.3870D 07	1.1610D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.8660D 06	3.8000D 12
3.60	3.8980D 08	8.5590D 09	1.4620D 07	1.1430D 09	4.5000D 12	3.8000D 17	4.0000D 09	1.9760D 06	3.8000D 12
3.80	3.8920D 08	8.5870D 09	1.5380D 07	1.1260D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.0910D 06	3.8000D 12
4.00	3.8870D 08	8.6150D 09	1.6130D 07	1.1090D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.2090D 06	3.8000D 12
4.20	3.8810D 08	8.6430D 09	1.6880D 07	1.0930D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.3310D 06	3.8000D 12
4.40	3.8760D 08	8.6700D 09	1.7630D 07	1.0760D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.4570D 06	3.8000D 12
4.60	3.8700D 08	8.6970D 09	1.8380D 07	1.0600D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.5850D 06	3.8000D 12
4.80	3.8650D 08	8.7240D 09	1.9130D 07	1.0440D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.7160D 06	3.8000D 12
5.00	3.8590D 08	8.7500D 09	1.9870D 07	1.0280D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.8500D 06	3.8000D 12
5.20	3.8540D 08	8.7760D 09	2.0610D 07	1.0130D 09	4.5000D 12	3.8000D 17	4.0000D 09	2.9860D 06	3.8000D 12
5.40	3.8480D 08	8.8020D 09	2.1350D 07	9.9780D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.1250D 06	3.8000D 12
5.60	3.8430D 08	8.8280D 09	2.2090D 07	9.8280D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.2650D 06	3.8000D 12
5.80	3.8370D 08	8.8530D 09	2.2820D 07	9.6800D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.4070D 06	3.8000D 12
6.00	3.8320D 08	8.8780D 09	2.3560D 07	9.5350D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.5510D 06	3.8000D 12
6.20	3.8260D 08	8.9030D 09	2.4290D 07	9.3910D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.6970D 06	3.8000D 12
6.40	3.8210D 08	8.9280D 09	2.5020D 07	9.2500D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.8430D 06	3.8000D 12
6.60	3.8150D 08	8.9520D 09	2.5750D 07	9.1110D 08	4.4990D 12	3.8000D 17	4.0000D 09	3.9910D 06	3.8000D 12
6.80	3.8100D 08	8.9760D 09	2.6480D 07	8.9740D 08	4.4990D 12	3.8000D 17	4.0000D 09	4.1410D 06	3.8000D 12
7.00	3.8040D 08	9.0000D 09	2.7200D 07	8.8380D 08	4.4990D 12	3.8000D 17	4.0000D 09	4.2910D 06	3.8000D 12
7.20	3.7990D 08	9.0240D 09	2.7930D 07	8.7050D 08	4.4990D 12	3.8000D 17	4.0000D 09	4.4410D 06	3.8000D 12
7.40	3.7940D 08	9.0470D 09	2.8650D 07	8.5740D 08	4.4990D 12	3.8000D 17	4.0000D 09	4.5930D 06	3.8000D 12
7.60	3.7880D 08	9.0710D 09	2.9380D 07	8.4450D 08	4.4990D 12	3.8000D 17	4.0000D 09	4.7450D 06	3.8000D 12
7.80	3.7830D 08	9.0940D 09	3.0100D 07	8.3180D 08	4.4990D 12	3.8000D 17	4.0000D 09	4.8980D 06	3.8000D 12
8.00	3.7770D 08	9.1170D 09	3.0820D 07	8.1920D 08	4.4990D 12	3.8000D 17	4.0000D 09	5.0510D 06	3.8000D 12
8.20	3.7720D 08	9.1390D 09	3.1540D 07	8.0690D 08	4.4990D 12	3.8000D 17	4.0010D 09	5.2050D 06	3.8000D 12
8.40	3.7670D 08	9.1610D 09	3.2260D 07	7.9470D 08	4.4990D 12	3.8000D 17	4.0010D 09	5.3590D 06	3.8000D 12
8.60	3.7610D 08	9.1840D 09	3.2970D 07	7.8270D 08	4.4990D 12	3.8000D 17	4.0010D 09	5.5130D 06	3.8000D 12
8.80	3.7560D 08	9.2060D 09	3.3690D 07	7.7090D 08	4.4990D 12	3.8000D 17	4.0010D 09	5.6670D 06	3.8000D 12
9.00	3.7510D 08	9.2270D 09	3.4410D 07	7.5930D 08	4.4990D 12	3.8000D 17	4.0010D 09	5.8210D 06	3.8000D 12
9.20	3.7450D 08	9.2490D 09	3.5120D 07	7.4780D 08	4.4990D 12	3.8000D 17	4.0010D 09	5.9760D 06	3.8000D 12
9.40	3.7400D 08	9.2700D 09	3.5840D 07	7.3650D 08	4.4990D 12	3.8000D 17	4.0010D 09	6.1300D 06	3.8000D 12
9.60	3.7350D 08	9.2910D 09	3.6550D 07	7.2540D 08	4.4990D 12	3.8000D 17	4.0010D 09	6.2840D 06	3.8000D 12
9.80	3.7300D 08	9.3120D 09	3.7260D 07	7.1440D 08	4.4990D 12	3.8000D 17	4.0010D 09	6.4380D 06	3.8000D 12
10.00	3.7240D 08	9.3330D 09	3.7970D 07	7.0360D 08	4.4990D 12	3.8000D 17	4.0010D 09	6.5910D 06	3.8000D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.000D 06	1.000D 06	1.000D 06	2.000D 07	1.300D 09	1.000D 06	1.000D 06	4.000D 09	1.000D 08
0.20	9.504D 01	7.294D-07	1.000D 06	3.220D 07	1.300D 09	1.000D 06	1.001D 06	3.989D 09	9.999D 07
0.40	9.504D 01	7.198D-07	1.000D 06	4.336D 07	1.300D 09	1.000D 06	1.001D 06	3.978D 09	9.998D 07
0.60	9.504D 01	7.191D-07	1.000D 06	5.448D 07	1.300D 09	1.000D 06	1.002D 06	3.967D 09	9.996D 07
0.80	9.504D 01	7.267D-07	1.000D 06	6.554D 07	1.300D 09	1.000D 06	1.002D 06	3.955D 09	9.995D 07
1.00	9.504D 01	7.422D-07	1.000D 06	7.656D 07	1.300D 09	1.000D 06	1.003D 06	3.944D 09	9.994D 07
1.20	9.504D 01	7.649D-07	1.000D 06	8.754D 07	1.300D 09	1.000D 06	1.003D 06	3.933D 09	9.993D 07
1.40	9.504D 01	7.946D-07	1.000D 06	9.847D 07	1.300D 09	1.000D 06	1.004D 06	3.922D 09	9.992D 07
1.60	9.504D 01	8.308D-07	1.000D 06	1.093D 08	1.300D 09	1.000D 06	1.005D 06	3.911D 09	9.990D 07
1.80	9.504D 01	8.730D-07	1.000D 06	1.202D 08	1.300D 09	1.000D 06	1.005D 06	3.901D 09	9.989D 07
2.00	9.504D 01	9.209D-07	1.000D 06	1.310D 08	1.300D 09	1.000D 06	1.006D 06	3.890D 09	9.988D 07
2.20	9.504D 01	9.742D-07	1.000D 06	1.417D 08	1.300D 09	1.000D 06	1.006D 06	3.879D 09	9.987D 07
2.40	9.504D 01	1.033D-06	1.000D 06	1.524D 08	1.300D 09	1.000D 06	1.007D 06	3.868D 09	9.986D 07
2.60	9.504D 01	1.095D-06	1.000D 06	1.631D 08	1.300D 09	1.000D 06	1.008D 06	3.857D 09	9.985D 07
2.80	9.505D 01	1.163D-06	1.000D 06	1.737D 08	1.300D 09	1.000D 06	1.009D 06	3.846D 09	9.983D 07
3.00	9.505D 01	1.234D-06	1.000D 06	1.843D 08	1.300D 09	1.000D 06	1.009D 06	3.836D 09	9.982D 07
3.20	9.505D 01	1.310D-06	1.000D 06	1.948D 08	1.300D 09	1.000D 06	1.010D 06	3.825D 09	9.981D 07
3.40	9.505D 01	1.388D-06	1.000D 06	2.053D 08	1.300D 09	1.000D 06	1.011D 06	3.814D 09	9.980D 07
3.60	9.505D 01	1.471D-06	1.000D 06	2.157D 08	1.300D 09	1.000D 06	1.012D 06	3.804D 09	9.979D 07
3.80	9.505D 01	1.556D-06	1.000D 06	2.261D 08	1.300D 09	1.000D 06	1.013D 06	3.793D 09	9.978D 07
4.00	9.506D 01	1.644D-06	1.000D 06	2.364D 08	1.300D 09	1.000D 06	1.014D 06	3.783D 09	9.977D 07
4.20	9.506D 01	1.735D-06	1.000D 06	2.468D 08	1.300D 09	1.000D 06	1.015D 06	3.772D 09	9.975D 07
4.40	9.506D 01	1.828D-06	1.000D 06	2.570D 08	1.300D 09	1.000D 06	1.016D 06	3.762D 09	9.974D 07
4.60	9.506D 01	1.923D-06	1.000D 06	2.672D 08	1.300D 09	1.000D 06	1.017D 06	3.751D 09	9.973D 07
4.80	9.507D 01	2.021D-06	1.000D 06	2.774D 08	1.300D 09	1.000D 06	1.018D 06	3.741D 09	9.972D 07
5.00	9.507D 01	2.121D-06	1.000D 06	2.875D 08	1.300D 09	1.000D 06	1.019D 06	3.730D 09	9.971D 07
5.20	9.508D 01	2.222D-06	1.000D 06	2.976D 08	1.301D 09	1.000D 06	1.021D 06	3.720D 09	9.970D 07
5.40	9.508D 01	2.325D-06	1.000D 06	3.077D 08	1.301D 09	1.000D 06	1.022D 06	3.710D 09	9.969D 07
5.60	9.508D 01	2.430D-06	1.000D 06	3.177D 08	1.301D 09	1.000D 06	1.023D 06	3.699D 09	9.968D 07
5.80	9.509D 01	2.536D-06	1.000D 06	3.276D 08	1.301D 09	1.000D 06	1.024D 06	3.689D 09	9.967D 07
6.00	9.509D 01	2.643D-06	1.000D 06	3.376D 08	1.301D 09	1.000D 06	1.026D 06	3.679D 09	9.965D 07
6.20	9.510D 01	2.751D-06	1.000D 06	3.474D 08	1.301D 09	1.000D 06	1.027D 06	3.669D 09	9.964D 07
6.40	9.511D 01	2.860D-06	1.000D 06	3.573D 08	1.301D 09	1.000D 06	1.029D 06	3.659D 09	9.963D 07
6.60	9.511D 01	2.970D-06	1.000D 06	3.670D 08	1.301D 09	1.000D 06	1.030D 06	3.648D 09	9.962D 07
6.80	9.512D 01	3.081D-06	1.000D 06	3.768D 08	1.301D 09	1.000D 06	1.032D 06	3.638D 09	9.961D 07
7.00	9.512D 01	3.193D-06	1.000D 06	3.865D 08	1.301D 09	1.000D 06	1.033D 06	3.628D 09	9.960D 07
7.20	9.513D 01	3.306D-06	1.000D 06	3.961D 08	1.301D 09	1.000D 06	1.035D 06	3.618D 09	9.959D 07
7.40	9.514D 01	3.419D-06	1.000D 06	4.057D 08	1.301D 09	1.000D 06	1.036D 06	3.608D 09	9.958D 07
7.60	9.515D 01	3.532D-06	1.000D 06	4.153D 08	1.302D 09	1.000D 06	1.038D 06	3.598D 09	9.957D 07
7.80	9.515D 01	3.646D-06	1.000D 06	4.248D 08	1.302D 09	1.000D 06	1.039D 06	3.588D 09	9.956D 07
8.00	9.516D 01	3.760D-06	1.000D 06	4.343D 08	1.302D 09	1.000D 06	1.041D 06	3.578D 09	9.955D 07
8.20	9.517D 01	3.875D-06	1.000D 06	4.438D 08	1.302D 09	1.000D 06	1.043D 06	3.568D 09	9.954D 07
8.40	9.518D 01	3.989D-06	1.000D 06	4.532D 08	1.302D 09	1.000D 06	1.044D 06	3.559D 09	9.952D 07
8.60	9.519D 01	4.104D-06	1.000D 06	4.625D 08	1.302D 09	1.000D 06	1.046D 06	3.549D 09	9.951D 07
8.80	9.520D 01	4.219D-06	1.000D 06	4.718D 08	1.302D 09	1.000D 06	1.048D 06	3.539D 09	9.950D 07
9.00	9.521D 01	4.334D-06	1.000D 06	4.811D 08	1.302D 09	1.000D 06	1.050D 06	3.529D 09	9.949D 07
9.20	9.521D 01	4.449D-06	1.000D 06	4.903D 08	1.303D 09	1.000D 06	1.052D 06	3.520D 09	9.948D 07
9.40	9.522D 01	4.564D-06	1.000D 06	4.995D 08	1.303D 09	1.000D 06	1.053D 06	3.510D 09	9.947D 07
9.60	9.523D 01	4.679D-06	1.000D 06	5.086D 08	1.303D 09	1.000D 06	1.055D 06	3.500D 09	9.946D 07
9.80	9.525D 01	4.794D-06	1.000D 06	5.177D 08	1.303D 09	1.000D 06	1.057D 06	3.491D 09	9.945D 07
10.00	9.526D 01	4.908D-06	1.000D 06	5.267D 08	1.303D 09	1.000D 06	1.059D 06	3.481D 09	9.944D 07

T=700 K, H= 20 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.06D 06	1.09D-14
2	2*NO3 >>> 2*NO2 + O2	2.57D-14	7.44D-49
3	NO2 + NO3 >>> NO2 + NO + O2	5.51D-14	3.97D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.23D-19
5	NO + O3 >>> NO2 + O2	2.65D-13	4.54D-28
6	NO2 + O3 >>> NO3 + O2	3.62D-15	6.56D-22
7	HNO3 + M >>> HO + NO2 + M	8.81D-02	1.47D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	4.74D-19
9	O + O + M >>> O2 + M	2.09D-16	3.01D-20
10	O + O2 + M >>> O3 + M	1.22D-16	7.38D 00
11	O + O3 >>> 2*O2	7.11D-13	8.63D-43
12	O + NO + M >>> NO2 + M	1.98D-14	4.70D-11
13	O + NO2 >>> NO + O2	1.11D-11	8.50D-27
14	O + NO2 + M >>> NO3 + M	5.56D-14	4.44D-24
15	HO + HO >>> H2O + O	4.53D-12	2.04D-16
16	O2 + 2*NO >>> 2*NO2	7.04D-39	9.37D-21
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.11D-15
19	O + HO2 >>> HO + O2	3.91D-11	2.19D-28
20	O2 + H + M >>> HO2 + M	6.05D-15	1.36D-05
21	O3 + H >>> HO + O2	4.78D-11	5.62D-37
22	O3 + HO >>> HO2 + O2	3.59D-13	8.31D-26
23	O3 + HO2 >>> HO + 2*O2	1.18D-14	1.12D-49
24	H + HO + M >>> H2O + M	3.06D-14	7.36D-27
25	H + HO2 >>> 2*HO	1.08D-10	5.87D-24
26	H + HO2 >>> H2 + O2	2.55D-11	8.03D-29
27	H + H2O >>> H2 + HO	6.56D-17	8.90D-13
28	H + H2O2 >>> H2 + HO2	3.06D-13	1.77D-18
29	H + H2O2 >>> HO + H2O	3.98D-13	1.02D-35

30	2*HO + M >>> H2O2 + M	2.51D-14	2.30D-04
31	HO + HO2 >>> H2O + O2	4.06D-11	7.73D-33
32	2*HO2 >>> H2O2 + O2	8.32D-12	3.02D-24
33	HO2 + H2O >>> H2O2 + HO	2.72D-21	3.07D-12
34	NO + H + M >>> HNO + M	6.40D-15	4.83D-06
35	NO + HO >>> NO2 + H	2.23D-21	2.02D-10
36	NO + HO + M >>> HNO2 + M	1.05D-13	1.30D-02
37	NO + HO2 >>> NO2 + HO	3.60D-12	2.68D-14
38	H + H + M >>> H2 + M	5.56D-16	4.65D-25
39	HNO4 + M >>> HO2 + NO2 + M	1.31D 06	1.23D-14
40	CLNO3 + M >>> CLO + NO2 + M	8.25D 05	5.49D-15

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.000D 08	8.000D 09	5.000D 05	1.500D 09	4.500D 12	3.800D 17	4.000D 09	1.000D 06	3.800D 12
0.20	2.277D-02	4.842D 09	4.574D 08	9.170D 09	3.422D 12	3.800D 17	3.930D 09	2.303D 09	3.800D 12
0.40	1.344D-02	2.799D 09	4.672D 08	1.127D 10	3.012D 12	3.800D 17	3.862D 09	2.372D 09	3.800D 12
0.60	1.082D-02	2.269D 09	4.639D 08	1.187D 10	2.688D 12	3.800D 17	3.794D 09	2.426D 09	3.800D 12
0.80	9.941D-03	2.119D 09	4.566D 08	1.210D 10	2.425D 12	3.800D 17	3.728D 09	2.471D 09	3.800D 12
1.00	9.556D-03	2.077D 09	4.476D 08	1.221D 10	2.207D 12	3.800D 17	3.663D 09	2.507D 09	3.800D 12
1.20	9.321D-03	2.071D 09	4.378D 08	1.229D 10	2.024D 12	3.800D 17	3.599D 09	2.536D 09	3.800D 12
1.40	9.132D-03	2.078D 09	4.276D 08	1.235D 10	1.868D 12	3.800D 17	3.536D 09	2.559D 09	3.800D 12
1.60	8.957D-03	2.090D 09	4.170D 08	1.241D 10	1.733D 12	3.800D 17	3.474D 09	2.576D 09	3.800D 12
1.80	8.784D-03	2.104D 09	4.062D 08	1.247D 10	1.616D 12	3.800D 17	3.414D 09	2.590D 09	3.800D 12
2.00	8.608D-03	2.118D 09	3.954D 08	1.253D 10	1.512D 12	3.800D 17	3.354D 09	2.599D 09	3.800D 12
2.20	8.431D-03	2.133D 09	3.846D 08	1.258D 10	1.421D 12	3.800D 17	3.295D 09	2.605D 09	3.800D 12
2.40	8.251D-03	2.148D 09	3.738D 08	1.263D 10	1.340D 12	3.800D 17	3.238D 09	2.608D 09	3.800D 12
2.60	8.069D-03	2.162D 09	3.631D 08	1.269D 10	1.266D 12	3.800D 17	3.181D 09	2.609D 09	3.800D 12
2.80	7.886D-03	2.177D 09	3.525D 08	1.274D 10	1.200D 12	3.800D 17	3.126D 09	2.607D 09	3.800D 12
3.00	7.702D-03	2.191D 09	3.421D 08	1.279D 10	1.141D 12	3.800D 17	3.071D 09	2.603D 09	3.800D 12
3.20	7.518D-03	2.205D 09	3.318D 08	1.284D 10	1.086D 12	3.800D 17	3.017D 09	2.598D 09	3.800D 12
3.40	7.335D-03	2.218D 09	3.217D 08	1.289D 10	1.036D 12	3.800D 17	2.965D 09	2.591D 09	3.800D 12
3.60	7.153D-03	2.232D 09	3.118D 08	1.293D 10	9.908D 11	3.800D 17	2.913D 09	2.582D 09	3.800D 12
3.80	6.971D-03	2.245D 09	3.022D 08	1.298D 10	9.487D 11	3.800D 17	2.862D 09	2.573D 09	3.800D 12
4.00	6.792D-03	2.258D 09	2.927D 08	1.303D 10	9.098D 11	3.800D 17	2.812D 09	2.562D 09	3.800D 12
4.20	6.615D-03	2.270D 09	2.835D 08	1.307D 10	8.738D 11	3.800D 17	2.763D 09	2.551D 09	3.800D 12
4.40	6.440D-03	2.282D 09	2.745D 08	1.312D 10	8.404D 11	3.800D 17	2.715D 09	2.539D 09	3.800D 12
4.60	6.267D-03	2.294D 09	2.658D 08	1.316D 10	8.092D 11	3.800D 17	2.668D 09	2.526D 09	3.800D 12
4.80	6.097D-03	2.306D 09	2.573D 08	1.320D 10	7.801D 11	3.800D 17	2.621D 09	2.512D 09	3.800D 12
5.00	5.930D-03	2.317D 09	2.491D 08	1.324D 10	7.529D 11	3.800D 17	2.575D 09	2.498D 09	3.800D 12
5.20	5.767D-03	2.328D 09	2.410D 08	1.328D 10	7.274D 11	3.800D 17	2.530D 09	2.484D 09	3.800D 12
5.40	5.606D-03	2.338D 09	2.333D 08	1.333D 10	7.035D 11	3.800D 17	2.486D 09	2.469D 09	3.800D 12
5.60	5.449D-03	2.349D 09	2.257D 08	1.337D 10	6.809D 11	3.800D 17	2.443D 09	2.454D 09	3.800D 12
5.80	5.295D-03	2.359D 09	2.184D 08	1.340D 10	6.597D 11	3.800D 17	2.400D 09	2.439D 09	3.800D 12
6.00	5.145D-03	2.369D 09	2.113D 08	1.344D 10	6.396D 11	3.800D 17	2.358D 09	2.423D 09	3.800D 12
6.20	4.998D-03	2.378D 09	2.045D 08	1.348D 10	6.207D 11	3.800D 17	2.317D 09	2.408D 09	3.801D 12
6.40	4.855D-03	2.388D 09	1.978D 08	1.352D 10	6.027D 11	3.800D 17	2.277D 09	2.392D 09	3.801D 12
6.60	4.715D-03	2.397D 09	1.914D 08	1.355D 10	5.856D 11	3.800D 17	2.237D 09	2.376D 09	3.801D 12
6.80	4.579D-03	2.406D 09	1.852D 08	1.359D 10	5.695D 11	3.800D 17	2.198D 09	2.360D 09	3.801D 12
7.00	4.447D-03	2.414D 09	1.792D 08	1.363D 10	5.541D 11	3.800D 17	2.160D 09	2.344D 09	3.801D 12
7.20	4.318D-03	2.423D 09	1.734D 08	1.366D 10	5.395D 11	3.800D 17	2.122D 09	2.328D 09	3.801D 12
7.40	4.193D-03	2.431D 09	1.678D 08	1.369D 10	5.255D 11	3.800D 17	2.085D 09	2.312D 09	3.801D 12
7.60	4.071D-03	2.439D 09	1.624D 08	1.373D 10	5.122D 11	3.800D 17	2.049D 09	2.296D 09	3.801D 12
7.80	3.953D-03	2.447D 09	1.572D 08	1.376D 10	4.995D 11	3.800D 17	2.013D 09	2.280D 09	3.801D 12
8.00	3.838D-03	2.454D 09	1.521D 08	1.379D 10	4.874D 11	3.800D 17	1.978D 09	2.264D 09	3.801D 12
8.20	3.726D-03	2.462D 09	1.473D 08	1.382D 10	4.758D 11	3.800D 17	1.943D 09	2.248D 09	3.801D 12
8.40	3.618D-03	2.469D 09	1.426D 08	1.385D 10	4.646D 11	3.800D 17	1.910D 09	2.232D 09	3.801D 12
8.60	3.513D-03	2.476D 09	1.381D 08	1.388D 10	4.540D 11	3.800D 17	1.876D 09	2.216D 09	3.801D 12
8.80	3.411D-03	2.482D 09	1.337D 08	1.391D 10	4.437D 11	3.800D 17	1.844D 09	2.200D 09	3.801D 12
9.00	3.313D-03	2.489D 09	1.295D 08	1.394D 10	4.339D 11	3.800D 17	1.811D 09	2.185D 09	3.801D 12
9.20	3.217D-03	2.495D 09	1.254D 08	1.397D 10	4.245D 11	3.800D 17	1.780D 09	2.169D 09	3.801D 12
9.40	3.125D-03	2.502D 09	1.215D 08	1.400D 10	4.154D 11	3.800D 17	1.749D 09	2.154D 09	3.801D 12
9.60	3.035D-03	2.508D 09	1.178D 08	1.403D 10	4.067D 11	3.800D 17	1.718D 09	2.138D 09	3.801D 12
9.80	2.949D-03	2.514D 09	1.141D 08	1.405D 10	3.983D 11	3.800D 17	1.689D 09	2.123D 09	3.801D 12
10.00	2.865D-03	2.519D 09	1.106D 08	1.408D 10	3.902D 11	3.800D 17	1.659D 09	2.108D 09	3.801D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.000D 06	1.000D 06	1.000D 06	2.000D 07	1.300D 09	1.000D 06	1.000D 06	4.000D 09	1.000D 08
0.20	5.223D 11	1.548D 07	1.130D 06	1.848D 09	1.307D 09	1.000D 06	1.252D 06	8.363D-02	4.345D-03
0.40	4.621D 11	1.419D 07	1.273D 06	1.909D 09	1.311D 09	1.000D 06	1.760D 06	4.993D-02	2.511D-03
0.60	4.139D 11	1.306D 07	1.409D 06	1.960D 09	1.316D 09	1.001D 06	2.339D 06	4.157D-02	2.036D-03
0.80	3.745D 11	1.208D 07	1.536D 06	2.002D 09	1.320D 09	1.001D 06	2.948D 06	3.964D-02	1.901D-03
1.00	3.417D 11	1.122D 07	1.657D 06	2.036D 09	1.325D 09	1.001D 06	3.573D 06	3.953D-02	1.864D-03
1.20	3.140D 11	1.046D 07	1.771D 06	2.063D 09	1.330D 09	1.001D 06	4.210D 06	3.995D-02	1.859D-03
1.40	2.902D 11	9.777D 06	1.878D 06	2.085D 09	1.335D 09	1.001D 06	4.856D 06	4.050D-02	1.865D-03
1.60	2.697D 11	9.167D 06	1.979D 06	2.102D 09	1.340D 09	1.001D 06	5.508D 06	4.106D-02	1.875D-03
1.80	2.518D 11	8.616D 06	2.075D 06	2.115D 09	1.345D 09	1.001D 06	6.166D 06	4.159D-02	1.888D-03
2.00	2.359D 11	8.117D 06	2.166D 06	2.124D 09	1.351D 09	1.002D 06	6.828D 06	4.206D-02	1.901D-03
2.20	2.219D 11	7.662D 06	2.251D 06	2.130D 09	1.356D 09	1.002D 06	7.494D 06	4.247D-02	1.914D-03
2.40	2.094D 11	7.246D 06	2.332D 06	2.134D 09	1.361D 09	1.002D 06	8.162D 06	4.283D-02	1.927D-03
2.60	1.981D 11	6.865D 06	2.408D 06	2.135D 09	1.367D 09	1.002D 06	8.831D 06	4.315D-02	1.940D-03
2.80	1.879D 11	6.514D 06	2.481D 06	2.134D 09	1.372D 09	1.002D 06	9.501D 06	4.342D-02	1.953D-03
3.00	1.787D 11	6.191D 06	2.550D 06	2.131D 09	1.377D 09	1.002D 06	1.017D 07	4.364D-02	1.966D-03
3.20	1.703D 11	5.891D 06	2.615D 06	2.127D 09	1.383D 09	1.002D 06	1.084D 07	4.383D-02	1.979D-03
3.40	1.625D 11	5.613D 06	2.677D 06	2.121D 09	1.388D 09	1.002D 06	1.151D 07	4.398D-02	1.991D-03
3.60	1.555D 11	5.355D 06	2.735D 06	2.114D 09	1.393D 09	1.002D 06	1.218D 07	4.410D-02	2.003D-03
3.80	1.489D 11	5.115D 06	2.791D 06	2.106D 09	1.398D 09	1.003D 06	1.285D 07	4.419D-02	2.014D-03
4.00	1.429D 11	4.890D 06	2.844D 06	2.097D 09	1.403D 09	1.003D 06	1.351D 07	4.425D-02	2.026D-03
4.20	1.373D 11	4.680D 06	2.894D 06	2.087D 09	1.408D 09	1.003D 06	1.417D 07	4.429D-02	2.037D-03
4.40	1.321D 11	4.483D 06	2.942D 06	2.077D 09	1.413D 09	1.003D 06	1.483D 07	4.430D-02	2.048D-03
4.60	1.272D 11	4.299D 06	2.988D 06	2.065D 09	1.418D 09	1.003D 06	1.549D 07	4.429D-02	2.059D-03
4.80	1.227D 11	4.126D 06	3.031D 06	2.054D 09	1.423D 09	1.003D 06	1.615D 07	4.426D-02	2.069D-03
5.00	1.185D 11	3.963D 06	3.072D 06	2.042D 09	1.428D 09	1.003D 06	1.680D 07	4.422D-02	2.079D-03
5.20	1.145D 11	3.809D 06	3.112D 06	2.029D 09	1.433D 09	1.003D 06	1.744D 07	4.416D-02	2.089D-03
5.40	1.107D 11	3.664D 06	3.149D 06	2.017D 09	1.437D 09	1.003D 06	1.809D 07	4.408D-02	2.098D-03
5.60	1.072D 11	3.527D 06	3.185D 06	2.003D 09	1.442D 09	1.003D 06	1.873D 07	4.399D-02	2.108D-03
5.80	1.039D 11	3.398D 06	3.220D 06	1.990D 09	1.446D 09	1.003D 06	1.936D 07	4.389D-02	2.117D-03
6.00	1.008D 11	3.275D 06	3.252D 06	1.977D 09	1.450D 09	1.003D 06	2.000D 07	4.377D-02	2.126D-03
6.20	9.781D 10	3.159D 06	3.284D 06	1.963D 09	1.455D 09	1.003D 06	2.062D 07	4.365D-02	2.134D-03
6.40	9.500D 10	3.049D 06	3.314D 06	1.949D 09	1.459D 09	1.003D 06	2.125D 07	4.351D-02	2.143D-03
6.60	9.233D 10	2.945D 06	3.342D 06	1.935D 09	1.463D 09	1.003D 06	2.187D 07	4.336D-02	2.151D-03
6.80	8.980D 10	2.845D 06	3.370D 06	1.921D 09	1.467D 09	1.004D 06	2.248D 07	4.321D-02	2.159D-03
7.00	8.739D 10	2.751D 06	3.396D 06	1.907D 09	1.471D 09	1.004D 06	2.309D 07	4.305D-02	2.167D-03
7.20	8.510D 10	2.661D 06	3.421D 06	1.893D 09	1.475D 09	1.004D 06	2.370D 07	4.288D-02	2.174D-03
7.40	8.291D 10	2.575D 06	3.445D 06	1.879D 09	1.479D 09	1.004D 06	2.430D 07	4.271D-02	2.182D-03
7.60	8.082D 10	2.493D 06	3.469D 06	1.865D 09	1.482D 09	1.004D 06	2.490D 07	4.253D-02	2.189D-03
7.80	7.883D 10	2.415D 06	3.491D 06	1.851D 09	1.486D 09	1.004D 06	2.549D 07	4.234D-02	2.196D-03
8.00	7.693D 10	2.341D 06	3.512D 06	1.837D 09	1.489D 09	1.004D 06	2.608D 07	4.215D-02	2.202D-03
8.20	7.511D 10	2.270D 06	3.532D 06	1.823D 09	1.493D 09	1.004D 06	2.666D 07	4.196D-02	2.209D-03
8.40	7.336D 10	2.202D 06	3.552D 06	1.810D 09	1.496D 09	1.004D 06	2.724D 07	4.176D-02	2.215D-03
8.60	7.169D 10	2.137D 06	3.571D 06	1.796D 09	1.500D 09	1.004D 06	2.782D 07	4.156D-02	2.222D-03
8.80	7.008D 10	2.074D 06	3.589D 06	1.782D 09	1.503D 09	1.004D 06	2.839D 07	4.135D-02	2.228D-03
9.00	6.854D 10	2.015D 06	3.606D 06	1.768D 09	1.506D 09	1.004D 06	2.895D 07	4.115D-02	2.234D-03
9.20	6.706D 10	1.957D 06	3.623D 06	1.755D 09	1.509D 09	1.004D 06	2.951D 07	4.094D-02	2.239D-03
9.40	6.564D 10	1.902D 06	3.639D 06	1.741D 09	1.512D 09	1.004D 06	3.007D 07	4.072D-02	2.245D-03
9.60	6.426D 10	1.850D 06	3.654D 06	1.728D 09	1.515D 09	1.004D 06	3.062D 07	4.051D-02	2.250D-03
9.80	6.294D 10	1.799D 06	3.669D 06	1.715D 09	1.518D 09	1.004D 06	3.116D 07	4.029D-02	2.256D-03
10.00	6.167D 10	1.750D 06	3.684D 06	1.702D 09	1.521D 09	1.004D 06	3.170D 07	4.008D-02	2.261D-03

T= 800 K, H=20 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	5.84D 06	8.15D-15
2	2*NO3 >>> 2*NO2 + O2	3.98D-14	5.95D-48
3	NO2 + NO3 >>> NO2 + NO + O2	6.59D-14	3.13D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.74D-18
5	NO + O3 >>> NO2 + O2	3.43D-13	4.42D-26
6	NO2 + O3 >>> NO3 + O2	5.61D-15	9.78D-21
7	HNO3 + M >>> HO + NO2 + M	4.18D 00	9.23D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.43D-18
9	O + O + M >>> O2 + M	1.56D-16	9.07D-16
10	O + O2 + M >>> O3 + M	9.75D-17	4.97D 01
11	O + O3 >>> 2*O2	1.07D-12	6.11D-39
12	O + NO + M >>> NO2 + M	1.56D-14	1.49D-08
13	O + NO2 >>> NO + O2	1.17D-11	5.55D-25
14	O + NO2 + M >>> NO3 + M	4.86D-14	3.89D-24
15	HO + HO >>> H2O + O	5.00D-12	1.06D-15
16	O2 + 2*NO >>> 2*NO2	6.40D-39	8.78D-20
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	9.55D-15
19	O + HO2 >>> HO + O2	4.28D-11	3.43D-26
20	O2 + H + M >>> HO2 + M	4.84D-15	7.22D-04
21	O3 + H >>> HO + O2	5.25D-11	6.31D-34
22	O3 + HO >>> HO2 + O2	4.30D-13	3.24D-24
23	O3 + HO2 >>> HO + 2*O2	1.48D-14	2.35D-48
24	H + HO + M >>> H2O + M	1.89D-14	1.87D-22
25	H + HO2 >>> 2*HO	1.28D-10	2.16D-22
26	H + HO2 >>> H2 + O2	2.71D-11	1.45D-26
27	H + H2O >>> H2 + HO	4.09D-16	1.41D-12
28	H + H2O2 >>> H2 + HO2	3.93D-13	9.47D-18
29	H + H2O2 >>> HO + H2O	5.11D-13	6.02D-33

30	2*HO + M >>> H2O2 + M	1.87D-14	1.54D-02
31	HO + HO2 >>> H2O + O2	4.44D-11	5.70D-30
32	2*HO2 >>> H2O2 + O2	9.10D-12	1.53D-22
33	HO2 + H2O >>> H2O2 + HO	5.19D-20	3.46D-12
34	NO + H + M >>> HNO + M	5.30D-15	3.15D-04
35	NO + HO >>> NO2 + H	3.30D-20	2.30D-10
36	NO + HO + M >>> HNO2 + M	7.51D-14	7.16D-01
37	NO + HO2 >>> NO2 + HO	4.46D-12	7.66D-14
38	H + H + M >>> H2 + M	4.86D-16	5.13D-21
39	HNO4 + M >>> HO2 + NO2 + M	6.97D 06	9.13D-15
40	CLNO3 + M >>> CLO + NO2 + M	5.34D 06	3.20D-15

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.000D 08	8.000D 09	5.000D 05	1.500D 09	4.500D 12	3.800D 17	4.000D 09	1.000D 06	3.800D 12
0.20	5.469D-04	8.662D 08	4.521D 08	1.535D 10	1.287D 12	3.800D 17	1.735D 09	6.922D 09	3.799D 12
0.40	3.999D-04	6.562D 08	4.364D 08	1.655D 10	9.539D 11	3.800D 17	7.528D 08	9.048D 09	3.798D 12
0.60	3.361D-04	5.783D 08	4.162D 08	1.708D 10	7.497D 11	3.800D 17	3.266D 08	1.017D 10	3.797D 12
0.80	2.939D-04	5.332D 08	3.947D 08	1.732D 10	6.124D 11	3.800D 17	1.417D 08	1.073D 10	3.797D 12
1.00	2.655D-04	5.095D 08	3.732D 08	1.745D 10	5.141D 11	3.800D 17	6.154D 07	1.098D 10	3.797D 12
1.20	2.455D-04	4.992D 08	3.522D 08	1.751D 10	4.404D 11	3.800D 17	2.676D 07	1.104D 10	3.797D 12
1.40	2.303D-04	4.967D 08	3.321D 08	1.755D 10	3.834D 11	3.800D 17	1.168D 07	1.098D 10	3.797D 12
1.60	2.178D-04	4.985D 08	3.129D 08	1.757D 10	3.381D 11	3.800D 17	5.132D 06	1.084D 10	3.797D 12
1.80	2.067D-04	5.025D 08	2.946D 08	1.759D 10	3.014D 11	3.800D 17	2.294D 06	1.066D 10	3.797D 12
2.00	1.966D-04	5.077D 08	2.773D 08	1.760D 10	2.710D 11	3.800D 17	1.062D 06	1.045D 10	3.797D 12
2.20	1.870D-04	5.132D 08	2.610D 08	1.761D 10	2.455D 11	3.800D 17	5.269D 05	1.022D 10	3.797D 12
2.40	1.779D-04	5.188D 08	2.455D 08	1.762D 10	2.239D 11	3.800D 17	2.940D 05	9.983D 09	3.797D 12
2.60	1.691D-04	5.243D 08	2.310D 08	1.763D 10	2.054D 11	3.800D 17	1.921D 05	9.743D 09	3.797D 12
2.80	1.607D-04	5.295D 08	2.173D 08	1.764D 10	1.893D 11	3.800D 17	1.470D 05	9.504D 09	3.798D 12
3.00	1.525D-04	5.345D 08	2.044D 08	1.765D 10	1.753D 11	3.800D 17	1.265D 05	9.270D 09	3.798D 12
3.20	1.447D-04	5.392D 08	1.922D 08	1.765D 10	1.630D 11	3.800D 17	1.166D 05	9.041D 09	3.798D 12
3.40	1.372D-04	5.437D 08	1.808D 08	1.766D 10	1.521D 11	3.800D 17	1.112D 05	8.818D 09	3.798D 12
3.60	1.301D-04	5.479D 08	1.700D 08	1.767D 10	1.424D 11	3.800D 17	1.079D 05	8.603D 09	3.798D 12
3.80	1.232D-04	5.518D 08	1.599D 08	1.767D 10	1.337D 11	3.800D 17	1.054D 05	8.395D 09	3.798D 12
4.00	1.166D-04	5.555D 08	1.504D 08	1.768D 10	1.259D 11	3.800D 17	1.033D 05	8.196D 09	3.798D 12
4.20	1.104D-04	5.590D 08	1.414D 08	1.768D 10	1.188D 11	3.800D 17	1.014D 05	8.004D 09	3.799D 12
4.40	1.044D-04	5.623D 08	1.330D 08	1.769D 10	1.124D 11	3.800D 17	9.962D 04	7.820D 09	3.799D 12
4.60	9.877D-05	5.654D 08	1.251D 08	1.770D 10	1.065D 11	3.800D 17	9.787D 04	7.644D 09	3.799D 12
4.80	9.339D-05	5.683D 08	1.177D 08	1.770D 10	1.012D 11	3.800D 17	9.617D 04	7.475D 09	3.799D 12
5.00	8.829D-05	5.711D 08	1.107D 08	1.770D 10	9.630D 10	3.800D 17	9.451D 04	7.312D 09	3.799D 12
5.20	8.345D-05	5.737D 08	1.042D 08	1.771D 10	9.179D 10	3.800D 17	9.290D 04	7.157D 09	3.799D 12
5.40	7.886D-05	5.761D 08	9.802D 07	1.771D 10	8.763D 10	3.800D 17	9.133D 04	7.008D 09	3.799D 12
5.60	7.452D-05	5.785D 08	9.225D 07	1.772D 10	8.378D 10	3.800D 17	8.980D 04	6.865D 09	3.799D 12
5.80	7.041D-05	5.807D 08	8.682D 07	1.772D 10	8.021D 10	3.800D 17	8.832D 04	6.728D 09	3.799D 12
6.00	6.652D-05	5.829D 08	8.173D 07	1.772D 10	7.689D 10	3.800D 17	8.688D 04	6.597D 09	3.800D 12
6.20	6.285D-05	5.849D 08	7.695D 07	1.773D 10	7.380D 10	3.800D 17	8.548D 04	6.471D 09	3.800D 12
6.40	5.938D-05	5.868D 08	7.247D 07	1.773D 10	7.091D 10	3.800D 17	8.413D 04	6.350D 09	3.800D 12
6.60	5.611D-05	5.887D 08	6.825D 07	1.773D 10	6.821D 10	3.800D 17	8.281D 04	6.233D 09	3.800D 12
6.80	5.302D-05	5.905D 08	6.430D 07	1.773D 10	6.568D 10	3.800D 17	8.154D 04	6.121D 09	3.800D 12
7.00	5.010D-05	5.922D 08	6.058D 07	1.774D 10	6.330D 10	3.800D 17	8.031D 04	6.014D 09	3.800D 12
7.20	4.735D-05	5.939D 08	5.710D 07	1.774D 10	6.107D 10	3.800D 17	7.912D 04	5.910D 09	3.800D 12
7.40	4.476D-05	5.955D 08	5.382D 07	1.774D 10	5.897D 10	3.800D 17	7.797D 04	5.810D 09	3.800D 12
7.60	4.231D-05	5.971D 08	5.075D 07	1.774D 10	5.698D 10	3.800D 17	7.685D 04	5.714D 09	3.800D 12
7.80	4.001D-05	5.986D 08	4.786D 07	1.774D 10	5.511D 10	3.800D 17	7.577D 04	5.622D 09	3.800D 12
8.00	3.783D-05	6.000D 08	4.515D 07	1.774D 10	5.334D 10	3.800D 17	7.472D 04	5.533D 09	3.800D 12
8.20	3.579D-05	6.015D 08	4.261D 07	1.775D 10	5.166D 10	3.800D 17	7.371D 04	5.446D 09	3.800D 12
8.40	3.386D-05	6.029D 08	4.022D 07	1.775D 10	5.007D 10	3.800D 17	7.273D 04	5.363D 09	3.800D 12
8.60	3.204D-05	6.042D 08	3.797D 07	1.775D 10	4.856D 10	3.800D 17	7.177D 04	5.283D 09	3.800D 12
8.80	3.033D-05	6.056D 08	3.587D 07	1.775D 10	4.712D 10	3.800D 17	7.085D 04	5.205D 09	3.801D 12
9.00	2.872D-05	6.069D 08	3.389D 07	1.775D 10	4.576D 10	3.800D 17	6.996D 04	5.130D 09	3.801D 12
9.20	2.720D-05	6.082D 08	3.203D 07	1.775D 10	4.446D 10	3.800D 17	6.910D 04	5.058D 09	3.801D 12
9.40	2.577D-05	6.095D 08	3.028D 07	1.775D 10	4.322D 10	3.800D 17	6.826D 04	4.988D 09	3.801D 12
9.60	2.443D-05	6.108D 08	2.864D 07	1.775D 10	4.204D 10	3.800D 17	6.745D 04	4.920D 09	3.801D 12
9.80	2.316D-05	6.120D 08	2.710D 07	1.775D 10	4.091D 10	3.800D 17	6.666D 04	4.854D 09	3.801D 12
10.00	2.197D-05	6.133D 08	2.565D 07	1.775D 10	3.982D 10	3.800D 17	6.590D 04	4.790D 09	3.801D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.0000D 07	1.3000D 09	1.0000D 06	1.0000D 06	4.0000D 09	1.0000 08
0.20	1.734D 12	9.105D 07	1.739D 06	2.231D 09	1.298D 09	1.001D 06	1.777D 06	2.529D-03	7.016D-05
0.40	1.282D 12	8.831D 07	3.067D 06	2.953D 09	1.300D 09	1.002D 06	3.369D 06	2.536D-03	5.315D-05
0.60	1.006D 12	7.805D 07	4.520D 06	3.333D 09	1.306D 09	1.004D 06	5.205D 06	2.523D-03	4.684D-05
0.80	8.214D 11	6.734D 07	5.889D 06	3.525D 09	1.314D 09	1.005D 06	7.040D 06	2.460D-03	4.318D-05
1.00	6.892D 11	5.786D 07	7.105D 06	3.607D 09	1.324D 09	1.006D 06	8.752D 06	2.405D-03	4.127D-05
1.20	5.903D 11	4.985D 07	8.159D 06	3.624D 09	1.334D 09	1.007D 06	1.028D 07	2.368D-03	4.043D-05
1.40	5.138D 11	4.317D 07	9.061D 06	3.601D 09	1.344D 09	1.008D 06	1.162D 07	2.341D-03	4.023D-05
1.60	4.530D 11	3.761D 07	9.831D 06	3.552D 09	1.353D 09	1.009D 06	1.275D 07	2.317D-03	4.038D-05
1.80	4.037D 11	3.296D 07	1.049D 07	3.488D 09	1.362D 09	1.009D 06	1.370D 07	2.294D-03	4.070D-05
2.00	3.630D 11	2.906D 07	1.105D 07	3.414D 09	1.370D 09	1.010D 06	1.447D 07	2.268D-03	4.112D-05
2.20	3.289D 11	2.576D 07	1.153D 07	3.334D 09	1.377D 09	1.010D 06	1.508D 07	2.239D-03	4.157D-05
2.40	2.999D 11	2.295D 07	1.194D 07	3.252D 09	1.383D 09	1.011D 06	1.556D 07	2.208D-03	4.202D-05
2.60	2.751D 11	2.055D 07	1.229D 07	3.169D 09	1.388D 09	1.011D 06	1.592D 07	2.174D-03	4.246D-05
2.80	2.536D 11	1.848D 07	1.260D 07	3.087D 09	1.393D 09	1.011D 06	1.617D 07	2.139D-03	4.289D-05
3.00	2.349D 11	1.670D 07	1.286D 07	3.006D 09	1.397D 09	1.011D 06	1.633D 07	2.103D-03	4.329D-05
3.20	2.184D 11	1.514D 07	1.309D 07	2.927D 09	1.400D 09	1.012D 06	1.641D 07	2.066D-03	4.367D-05
3.40	2.038D 11	1.378D 07	1.329D 07	2.850D 09	1.402D 09	1.012D 06	1.643D 07	2.028D-03	4.404D-05
3.60	1.908D 11	1.259D 07	1.346D 07	2.776D 09	1.404D 09	1.012D 06	1.639D 07	1.991D-03	4.437D-05
3.80	1.791D 11	1.154D 07	1.361D 07	2.705D 09	1.405D 09	1.012D 06	1.631D 07	1.954D-03	4.469D-05
4.00	1.686D 11	1.060D 07	1.375D 07	2.637D 09	1.406D 09	1.012D 06	1.618D 07	1.917D-03	4.499D-05
4.20	1.592D 11	9.776D 06	1.386D 07	2.571D 09	1.406D 09	1.013D 06	1.603D 07	1.881D-03	4.528D-05
4.40	1.506D 11	9.036D 06	1.397D 07	2.508D 09	1.406D 09	1.013D 06	1.585D 07	1.845D-03	4.554D-05
4.60	1.428D 11	8.374D 06	1.406D 07	2.447D 09	1.406D 09	1.013D 06	1.565D 07	1.811D-03	4.579D-05
4.80	1.356D 11	7.778D 06	1.413D 07	2.389D 09	1.405D 09	1.013D 06	1.543D 07	1.777D-03	4.603D-05
5.00	1.290D 11	7.241D 06	1.420D 07	2.334D 09	1.404D 09	1.013D 06	1.521D 07	1.744D-03	4.625D-05
5.20	1.230D 11	6.756D 06	1.427D 07	2.281D 09	1.402D 09	1.013D 06	1.497D 07	1.712D-03	4.646D-05
5.40	1.174D 11	6.316D 06	1.432D 07	2.229D 09	1.401D 09	1.013D 06	1.473D 07	1.681D-03	4.667D-05
5.60	1.123D 11	5.916D 06	1.437D 07	2.181D 09	1.399D 09	1.013D 06	1.448D 07	1.651D-03	4.686D-05
5.80	1.075D 11	5.551D 06	1.441D 07	2.134D 09	1.396D 09	1.013D 06	1.424D 07	1.622D-03	4.704D-05
6.00	1.030D 11	5.218D 06	1.445D 07	2.089D 09	1.394D 09	1.013D 06	1.399D 07	1.593D-03	4.721D-05
6.20	9.889D 10	4.912D 06	1.448D 07	2.045D 09	1.391D 09	1.013D 06	1.374D 07	1.566D-03	4.737D-05
6.40	9.503D 10	4.632D 06	1.451D 07	2.004D 09	1.388D 09	1.013D 06	1.350D 07	1.539D-03	4.753D-05
6.60	9.141D 10	4.374D 06	1.453D 07	1.964D 09	1.385D 09	1.013D 06	1.326D 07	1.513D-03	4.768D-05
6.80	8.802D 10	4.137D 06	1.455D 07	1.926D 09	1.382D 09	1.013D 06	1.302D 07	1.488D-03	4.783D-05
7.00	8.484D 10	3.917D 06	1.457D 07	1.889D 09	1.379D 09	1.013D 06	1.279D 07	1.464D-03	4.797D-05
7.20	8.185D 10	3.714D 06	1.459D 07	1.853D 09	1.375D 09	1.013D 06	1.257D 07	1.441D-03	4.810D-05
7.40	7.903D 10	3.526D 06	1.460D 07	1.819D 09	1.372D 09	1.013D 06	1.234D 07	1.418D-03	4.823D-05
7.60	7.638D 10	3.351D 06	1.461D 07	1.786D 09	1.368D 09	1.013D 06	1.213D 07	1.396D-03	4.836D-05
7.80	7.387D 10	3.189D 06	1.462D 07	1.755D 09	1.364D 09	1.013D 06	1.192D 07	1.374D-03	4.848D-05
8.00	7.150D 10	3.037D 06	1.463D 07	1.724D 09	1.360D 09	1.013D 06	1.171D 07	1.354D-03	4.860D-05
8.20	6.925D 10	2.896D 06	1.463D 07	1.694D 09	1.357D 09	1.013D 06	1.151D 07	1.334D-03	4.872D-05
8.40	6.712D 10	2.764D 06	1.464D 07	1.666D 09	1.353D 09	1.013D 06	1.132D 07	1.314D-03	4.883D-05
8.60	6.509D 10	2.641D 06	1.464D 07	1.638D 09	1.348D 09	1.013D 06	1.113D 07	1.296D-03	4.894D-05
8.80	6.317D 10	2.525D 06	1.464D 07	1.612D 09	1.344D 09	1.013D 06	1.095D 07	1.277D-03	4.905D-05
9.00	6.134D 10	2.417D 06	1.464D 07	1.586D 09	1.340D 09	1.013D 06	1.077D 07	1.260D-03	4.916D-05
9.20	5.960D 10	2.315D 06	1.464D 07	1.561D 09	1.336D 09	1.013D 06	1.060D 07	1.243D-03	4.926D-05
9.40	5.794D 10	2.219D 06	1.464D 07	1.537D 09	1.331D 09	1.013D 06	1.044D 07	1.226D-03	4.937D-05
9.60	5.635D 10	2.129D 06	1.464D 07	1.513D 09	1.327D 09	1.013D 06	1.027D 07	1.210D-03	4.947D-05
9.80	5.484D 10	2.044D 06	1.464D 07	1.491D 09	1.323D 09	1.013D 06	1.012D 07	1.194D-03	4.957D-05
10.00	5.339D 10	1.964D 06	1.464D 07	1.469D 09	1.318D 09	1.013D 06	9.966D 06	1.179D-03	4.967D-05

T= 250 K, H= 25 km 19 torr

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	4.05D-06	1.27D-13
2	2*NO3 >>> 2*NO2 + O2	4.71D-17	7.46D-62
3	NO2 + NO3 >>> NO2 + NO + O2	4.21D-15	1.19D-34
4	NO3 + NO >>> 2*NO2	1.90D-11	3.29D-32
5	NO + O3 >>> NO2 + O2	6.36D-15	1.08D-56
6	NO2 + O3 >>> NO3 + O2	6.65D-18	8.33D-39
7	HNO3 + M >>> HO + NO2 + M	5.36D-28	2.46D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.80D-29
9	O + O + M >>> O2 + M	2.69D-15	1.44D-57
10	O + O2 + M >>> O3 + M	5.76D-16	1.62D-12
11	O + O3 >>> 2*O2	1.92D-15	0.0
12	O + NO + M >>> NO2 + M	1.13D-13	8.39D-48
13	O + NO2 >>> NO + O2	5.12D-12	6.27D-53
14	O + NO2 + M >>> NO3 + M	7.07D-14	5.66D-24
15	HO + HO >>> H2O + O	1.09D-12	9.77D-27
16	O2 + 2*NO >>> 2*NO2	2.75D-38	3.88D-35
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	7.73D-25
19	O + HO2 >>> HO + O2	1.08D-11	5.45D-60
20	O2 + H + M >>> HO2 + M	2.78D-14	3.57D-31
21	O3 + H >>> HO + O2	1.27D-11	0.0
22	O3 + HO >>> HO2 + O2	2.75D-14	1.04D-48
23	O3 + HO2 >>> HO + 2*O2	4.45D-16	2.41D-68
24	H + HO + M >>> H2O + M	5.67D-13	0.0
25	H + HO2 >>> 2*HO	9.40D-12	1.62D-46
26	H + HO2 >>> H2 + O2	1.04D-11	2.55D-61
27	H + H2O >>> H2 + HO	2.34D-28	1.14D-15
28	H + H2O2 >>> H2 + HO2	8.36D-15	5.62D-29
29	H + H2O2 >>> HO + H2O	1.09D-14	1.35D-75

30	2*HO + M >>> H2O2 + M	3.23D-13	8.68D-32
31	HO + HO2 >>> H2O + O2	1.12D-11	3.89D-74
32	2*HO2 >>> H2O2 + O2	2.30D-12	8.58D-49
33	HO2 + H2O >>> H2O2 + HO	1.02D-39	5.49D-13
34	NO + H + M >>> HNO + M	1.76D-14	2.75D-33
35	NO + HO >>> NO2 + H	3.05D-38	3.01D-11
36	NO + HO + M >>> HNO2 + M	2.31D-12	8.77D-29
37	NO + HO2 >>> NO2 + HO	1.65D-13	7.47D-21
38	H + H + M >>> H2 + M	7.07D-16	0.0
39	HNO4 + M >>> HO2 + NO2 + M	1.09D-05	2.02D-13
40	CLNO3 + M >>> CLO + NO2 + M	3.26D-07	1.59D-13

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	7.0000D 08	6.5000D 09	2.0000D 06	7.0000D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.5000D 06	1.9000D 12
0.20	7.0000D 08	6.5040D 09	2.0310D 06	6.9630D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4800D 06	1.9000D 12
0.40	7.0000D 08	6.5070D 09	2.0630D 06	6.9260D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4510D 06	1.9000D 12
0.60	7.0000D 08	6.5110D 09	2.0940D 06	6.8890D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4220D 06	1.9000D 12
0.80	7.0000D 08	6.5150D 09	2.1250D 06	6.8520D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3930D 06	1.9000D 12
1.00	7.0000D 08	6.5180D 09	2.1560D 06	6.8150D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3660D 06	1.9000D 12
1.20	7.0000D 08	6.5220D 09	2.1870D 06	6.7790D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3390D 06	1.9000D 12
1.40	7.0000D 08	6.5250D 09	2.2180D 06	6.7430D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3130D 06	1.9000D 12
1.60	7.0000D 08	6.5290D 09	2.2490D 06	6.7070D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.2870D 06	1.9000D 12
1.80	7.0000D 08	6.5320D 09	2.2800D 06	6.6710D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.2630D 06	1.9000D 12
2.00	7.0000D 08	6.5360D 09	2.3110D 06	6.6350D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.2390D 06	1.9000D 12
2.20	7.0000D 08	6.5400D 09	2.3420D 06	6.6000D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.2150D 06	1.9000D 12
2.40	7.0000D 08	6.5430D 09	2.3730D 06	6.5650D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.1930D 06	1.9000D 12
2.60	7.0000D 08	6.5460D 09	2.4040D 06	6.5300D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.1700D 06	1.9000D 12
2.80	7.0000D 08	6.5500D 09	2.4350D 06	6.4950D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.1490D 06	1.9000D 12
3.00	7.0000D 08	6.5530D 09	2.4650D 06	6.4600D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.1280D 06	1.9000D 12
3.20	7.0000D 08	6.5570D 09	2.4960D 06	6.4260D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.1070D 06	1.9000D 12
3.40	7.0000D 08	6.5600D 09	2.5270D 06	6.3910D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.0870D 06	1.9000D 12
3.60	7.0000D 08	6.5630D 09	2.5580D 06	6.3570D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.0680D 06	1.9000D 12
3.80	7.0000D 08	6.5670D 09	2.5880D 06	6.3230D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.0490D 06	1.9000D 12
4.00	7.0000D 08	6.5700D 09	2.6190D 06	6.2900D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.0310D 06	1.9000D 12
4.20	7.0000D 08	6.5730D 09	2.6500D 06	6.2560D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.0130D 06	1.9000D 12
4.40	7.0000D 08	6.5770D 09	2.6800D 06	6.2230D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.9570D 05	1.9000D 12
4.60	7.0000D 08	6.5800D 09	2.7110D 06	6.1890D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.7880D 05	1.9000D 12
4.80	7.0000D 08	6.5830D 09	2.7410D 06	6.1560D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.6240D 05	1.9000D 12
5.00	7.0000D 08	6.5870D 09	2.7720D 06	6.1240D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.4630D 05	1.9000D 12
5.20	7.0000D 08	6.5900D 09	2.8020D 06	6.0910D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.3070D 05	1.9000D 12
5.40	7.0000D 08	6.5930D 09	2.8330D 06	6.0580D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.1560D 05	1.9000D 12
5.60	7.0000D 08	6.5960D 09	2.8630D 06	6.0260D 08	4.2000D 12	1.7000D 17	2.0000D 09	9.0080D 05	1.9000D 12
5.80	7.0000D 08	6.5990D 09	2.8940D 06	5.9940D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.8640D 05	1.9000D 12
6.00	7.0000D 08	6.6020D 09	2.9240D 06	5.9620D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.7240D 05	1.9000D 12
6.20	7.0000D 08	6.6060D 09	2.9540D 06	5.9300D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.5880D 05	1.9000D 12
6.40	7.0000D 08	6.6090D 09	2.9850D 06	5.8980D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.4550D 05	1.9000D 12
6.60	7.0000D 08	6.6120D 09	3.0150D 06	5.8670D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.3260D 05	1.9000D 12
6.80	7.0000D 08	6.6150D 09	3.0450D 06	5.8360D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.2010D 05	1.9000D 12
7.00	7.0000D 08	6.6180D 09	3.0760D 06	5.8040D 08	4.2000D 12	1.7000D 17	2.0000D 09	8.0780D 05	1.9000D 12
7.20	7.0000D 08	6.6210D 09	3.1060D 06	5.7730D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.9590D 05	1.9000D 12
7.40	7.0000D 08	6.6240D 09	3.1360D 06	5.7430D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.8430D 05	1.9000D 12
7.60	7.0000D 08	6.6270D 09	3.1660D 06	5.7120D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.7310D 05	1.9000D 12
7.80	7.0000D 08	6.6300D 09	3.1970D 06	5.6810D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.6210D 05	1.9000D 12
8.00	7.0000D 08	6.6330D 09	3.2270D 06	5.6510D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.5140D 05	1.9000D 12
8.20	7.0000D 08	6.6360D 09	3.2570D 06	5.6210D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.4100D 05	1.9000D 12
8.40	7.0000D 08	6.6390D 09	3.2870D 06	5.5910D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.3090D 05	1.9000D 12
8.60	7.0000D 08	6.6420D 09	3.3170D 06	5.5610D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.2100D 05	1.9000D 12
8.80	7.0000D 08	6.6450D 09	3.3470D 06	5.5310D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.1140D 05	1.9000D 12
9.00	7.0000D 08	6.6480D 09	3.3780D 06	5.5020D 08	4.2000D 12	1.7000D 17	2.0000D 09	7.0210D 05	1.9000D 12
9.20	7.0000D 08	6.6510D 09	3.4080D 06	5.4720D 08	4.2000D 12	1.7000D 17	2.0000D 09	6.9300D 05	1.9000D 12
9.40	7.0000D 08	6.6540D 09	3.4380D 06	5.4430D 08	4.2000D 12	1.7000D 17	2.0000D 09	6.8420D 05	1.9000D 12
9.60	7.0000D 08	6.6560D 09	3.4680D 06	5.4140D 08	4.2000D 12	1.7000D 17	2.0000D 09	6.7550D 05	1.9000D 12
9.80	7.0000D 08	6.6590D 09	3.4980D 06	5.3850D 08	4.2000D 12	1.7000D 17	2.0000D 09	6.6720D 05	1.9000D 12
10.00	7.0000D 08	6.6620D 09	3.5280D 06	5.3560D 08	4.2000D 12	1.7000D 17	2.0000D 09	6.5900D 05	1.9000D 12

TIME(S)	O	H	HO	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.3000D 07	1.8000D 09	1.0000D 06	8.0000D 05	3.5000D 09	4.0000D 08
0.20	9.6610D-02	3.5390D-07	1.0000D 06	2.4010D 07	1.8000D 09	1.0000D 06	8.0050D 05	3.5000D 09	4.0000D 08
0.40	9.2580D-02	3.4670D-07	1.0000D 06	2.4040D 07	1.8000D 09	1.0000D 06	8.0100D 05	3.5000D 09	4.0000D 08
0.60	9.1660D-02	3.3970D-07	1.0000D 06	2.4060D 07	1.8000D 09	1.0000D 06	8.0140D 05	3.5000D 09	4.0000D 08
0.80	9.0770D-02	3.3300D-07	1.0000D 06	2.4090D 07	1.8000D 09	1.0000D 06	8.0190D 05	3.5000D 09	4.0000D 08
1.00	8.9930D-02	3.2640D-07	1.0000D 06	2.4110D 07	1.8000D 09	1.0000D 06	8.0230D 05	3.5000D 09	4.0010D 08
1.20	8.9120D-02	3.2000D-07	1.0000D 06	2.4130D 07	1.8000D 09	1.0000D 06	8.0270D 05	3.5000D 09	4.0010D 08
1.40	8.8360D-02	3.1370D-07	1.0000D 06	2.4160D 07	1.8000D 09	1.0000D 06	8.0310D 05	3.5000D 09	4.0010D 08
1.60	8.7620D-02	3.0770D-07	1.0000D 06	2.4180D 07	1.8000D 09	1.0000D 06	8.0350D 05	3.5000D 09	4.0010D 08
1.80	8.6920D-02	3.0170D-07	1.0000D 06	2.4200D 07	1.8000D 09	1.0000D 06	8.0390D 05	3.5000D 09	4.0010D 08
2.00	8.6260D-02	2.9600D-07	1.0000D 06	2.4220D 07	1.8000D 09	1.0000D 06	8.0430D 05	3.5000D 09	4.0010D 08
2.20	8.5620D-02	2.9040D-07	1.0000D 06	2.4240D 07	1.8000D 09	1.0000D 06	8.0470D 05	3.5000D 09	4.0010D 08
2.40	8.5010D-02	2.8490D-07	1.0000D 06	2.4260D 07	1.8000D 09	1.0000D 06	8.0510D 05	3.5000D 09	4.0010D 08
2.60	8.4430D-02	2.7960D-07	1.0000D 06	2.4280D 07	1.8000D 09	1.0000D 06	8.0540D 05	3.5000D 09	4.0020D 08
2.80	8.3870D-02	2.7450D-07	1.0000D 06	2.4290D 07	1.8000D 09	1.0000D 06	8.0580D 05	3.5000D 09	4.0020D 08
3.00	8.3340D-02	2.6950D-07	1.0000D 06	2.4310D 07	1.8000D 09	1.0000D 06	8.0610D 05	3.5000D 09	4.0020D 08
3.20	8.2830D-02	2.6460D-07	1.0000D 06	2.4330D 07	1.8000D 09	1.0000D 06	8.0640D 05	3.5000D 09	4.0020D 08
3.40	8.2350D-02	2.5980D-07	1.0000D 06	2.4350D 07	1.8000D 09	1.0000D 06	8.0680D 05	3.5000D 09	4.0020D 08
3.60	8.1880D-02	2.5520D-07	1.0000D 06	2.4360D 07	1.8000D 09	1.0000D 06	8.0710D 05	3.5000D 09	4.0020D 08
3.80	8.1440D-02	2.5070D-07	1.0000D 06	2.4380D 07	1.8000D 09	1.0000D 06	8.0740D 05	3.5000D 09	4.0020D 08
4.00	8.1020D-02	2.4630D-07	1.0000D 06	2.4390D 07	1.8000D 09	1.0000D 06	8.0770D 05	3.5000D 09	4.0020D 08
4.20	8.0610D-02	2.4200D-07	1.0000D 06	2.4410D 07	1.8000D 09	1.0000D 06	8.0800D 05	3.5000D 09	4.0020D 08
4.40	8.0220D-02	2.3790D-07	1.0000D 06	2.4420D 07	1.8000D 09	1.0000D 06	8.0830D 05	3.5000D 09	4.0030D 08
4.60	7.9850D-02	2.3380D-07	1.0000D 06	2.4440D 07	1.8000D 09	1.0000D 06	8.0860D 05	3.5000D 09	4.0030D 08
4.80	7.9500D-02	2.2990D-07	1.0000D 06	2.4450D 07	1.8000D 09	1.0000D 06	8.0890D 05	3.5000D 09	4.0030D 08
5.00	7.9160D-02	2.2610D-07	1.0000D 06	2.4460D 07	1.8000D 09	1.0000D 06	8.0910D 05	3.5000D 09	4.0030D 08
5.20	7.8830D-02	2.2230D-07	1.0000D 06	2.4470D 07	1.8000D 09	1.0000D 06	8.0940D 05	3.5000D 09	4.0030D 08
5.40	7.8520D-02	2.1870D-07	1.0000D 06	2.4490D 07	1.8000D 09	1.0000D 06	8.0960D 05	3.5000D 09	4.0030D 08
5.60	7.8220D-02	2.1520D-07	1.0000D 06	2.4500D 07	1.8000D 09	1.0000D 06	8.0990D 05	3.5000D 09	4.0030D 08
5.80	7.7940D-02	2.1170D-07	1.0000D 06	2.4510D 07	1.8000D 09	1.0000D 06	8.1010D 05	3.5000D 09	4.0030D 08
6.00	7.7670D-02	2.0840D-07	1.0000D 06	2.452[illegible]D 07	1.8000D 09	1.0000D 06	8.1040D 05	3.5000D 09	4.0040D 08
6.20	7.7400D-02	2.0510D-07	1.0000D 06	2.4530D 07	1.8000D 09	1.0000D 06	8.1060D 05	3.5000D 09	4.0040D 08
6.40	7.7150D-02	2.0200D-07	1.0000D 06	2.4540D 07	1.8000D 09	1.0000D 06	8.1090D 05	3.5000D 09	4.0040D 08
6.60	7.6910D-02	1.9890D-07	1.0000D 06	2.4550D 07	1.8000D 09	1.0000D 06	8.1110D 05	3.5000D 09	4.0040D 08
6.80	7.6680D-02	1.9590D-07	1.0000D 06	2.4560D 07	1.8000D 09	1.0000D 06	8.1130D 05	3.5000D 09	4.0040D 08
7.00	7.6460D-02	1.9300D-07	1.0000D 06	2.4570D 07	1.8000D 09	1.0000D 06	8.1150D 05	3.5000D 09	4.0040D 08
7.20	7.6250D-02	1.9010D-07	1.0000D 06	2.4580D 07	1.8000D 09	1.0000D 06	8.1170D 05	3.5000D 09	4.0040D 08
7.40	7.6050D-02	1.8730D-07	1.0000D 06	2.4590D 07	1.8000D 09	1.0000D 06	8.1200D 05	3.5000D 09	4.0040D 08
7.60	7.5850D-02	1.8470D-07	1.0000D 06	2.4600D 07	1.8000D 09	1.0000D 06	8.1220D 05	3.5000D 09	4.0050D 08
7.80	7.5660D-02	1.8200D-07	1.0000D 06	2.4610D 07	1.8000D 09	1.0000D 06	8.1240D 05	3.5000D 09	4.0050D 08
8.00	7.5480D-02	1.7950D-07	1.0000D 06	2.4620D 07	1.8000D 09	1.0000D 06	8.1260D 05	3.5000D 09	4.0050D 08
8.20	7.5310D-02	1.7700D-07	1.0000D 06	2.4630D 07	1.8000D 09	1.0000D 06	8.1280D 05	3.5000D 09	4.0050D 08
8.40	7.5150D-02	1.7460D-07	1.0000D 06	2.4630D 07	1.8000D 09	1.0000D 06	8.1300D 05	3.5000D 09	4.0050D 08
8.60	7.4990D-02	1.7220D-07	1.0000D 06	2.4640D 07	1.8000D 09	1.0000D 06	8.1310D 05	3.5000D 09	4.0050D 08
8.80	7.4830D-02	1.6990D-07	1.0000D 06	2.4650D 07	1.8000D 09	1.0000D 06	8.1330D 05	3.5000D 09	4.0050D 08
9.00	7.4690D-02	1.6770D-07	1.0000D 06	2.4660D 07	1.8000D 09	1.0000D 06	8.1350D 05	3.5000D 09	4.0050D 08
9.20	7.4550D-02	1.6550D-07	1.0000D 06	2.4660D 07	1.8000D 09	1.0000D 06	8.1370D 05	3.5000D 09	4.0050D 08
9.40	7.4410D-02	1.6340D-07	1.0000D 06	2.4670D 07	1.8000D 09	1.0000D 06	8.1390D 05	3.5000D 09	4.0060D 08
9.60	7.4280D-02	1.6130D-07	1.0000D 06	2.4680D 07	1.8000D 09	1.0000D 06	8.1400D 05	3.5000D 09	4.0060D 08
9.80	7.4160D-02	1.5930D-07	1.0000D 06	2.4680D 07	1.8000D 09	1.0000D 06	8.1420D 05	3.5000D 09	4.0060D 08
10.00	7.4040D-02	1.5740D-07	1.0000D 06	2.4690D 07	1.8000D 09	1.0000D 06	8.1440D 05	3.5000D 09	4.0060D 08

T=300 K, H= 25 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	3.27D-03	5.94D-14
2	2*NO3 >>> 2*NO2 + O2	2.41D-16	1.75D-58
3	NO2 + NO3 >>> NO2 + NO + O2	8.21D-15	4.92D-35
4	NO3 + NO >>> 2*NO2	1.90D-11	6.98D-29
5	NO + O3 >>> NO2 + O2	1.67D-14	2.85D-49
6	NO2 + O3 >>> NO3 + O2	3.41D-17	2.00D-34
7	HNO3 + M >>> HO + NO2 + M	4.01D-21	1.30D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	1.25D-26
9	O + O + M >>> O2 + M	1.23D-15	5.48D-58
10	O + O2 + M >>> O3 + M	3.42D-16	2.74D-09
11	O + O3 >>> 2*O2	8.90D-15	0.0
12	O + NO + M >>> NO2 + M	6.40D-14	2.51D-38
13	O + NO2 >>> NO + O2	6.25D-12	3.73D-46
14	O + NO2 + M >>> NO3 + M	5.89D-14	4.71D-24
15	HO + HO >>> H2O + O	1.57D-12	4.63D-24
16	O2 + 2*NO >>> 2*NO2	1.93D-38	2.26D-31
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.16D-22
19	O + HO2 >>> HO + O2	1.51D-11	8.51D-52
20	O2 + H + M >>> HO2 + M	1.66D-14	1.36D-24
21	O3 + H >>> HO + O2	1.79D-11	1.62D-69
22	O3 + HO >>> HO2 + O2	5.35D-14	8.98D-43
23	O3 + HO2 >>> HO + 2*O2	1.04D-15	1.53D-63
24	H + HO + M >>> H2O + M	2.94D-13	2.38D-75
25	H + HO2 >>> 2*HO	1.77D-11	1.14D-40
26	H + HO2 >>> H2 + O2	1.31D-11	6.80D-53
27	H + H2O >>> H2 + HO	2.18D-25	6.41D-15
28	H + H2O2 >>> H2 + HO2	2.13D-14	2.96D-26
29	H + H2O2 >>> HO + H2O	2.76D-14	2.95D-65

30	2*HO + M >>> H2O2 + M	1.480-13	1.080-24
31	HO + HO2 >>> H2O + O2	1.570-11	1.980-63
32	2*HO2 >>> H2O2 + O2	4.210-12	1.940-42
33	HO2 + H2O >>> H2O2 + HO	6.110-35	8.570-13
34	NO + H + M >>> HNO + M	1.200-14	3.080-26
35	NO + HO >>> NO2 + H	7.190-34	4.920-11
36	NO + HO + M >>> HNO2 + M	9.200-13	5.170-22
37	NO + HO2 >>> NO2 + HO	3.660-13	3.740-19
38	H + H + M >>> H2 + M	5.890-16	5.070-69
39	HNO4 + M >>> HO2 + NO2 + M	7.360-03	8.820-14
40	CLNO3 + M >>> CLO + NO2 + M	4.760-04	7.770-14

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	7.0000D 08	6.5000D 09	2.0000D 06	7.0000D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.5000D 06	1.9000D 12
0.20	6.9950D 08	6.5150D 09	2.6380D 06	6.9020D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4800D 06	1.9000D 12
0.40	6.9910D 08	6.5300D 09	3.2750D 06	6.8060D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4400D 06	1.9000D 12
0.60	6.9860D 08	6.5450D 09	3.9100D 06	6.7110D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4070D 06	1.9000D 12
0.80	6.9820D 08	6.5600D 09	4.5440D 06	6.6170D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3800D 06	1.9000D 12
1.00	6.9770D 08	6.5750D 09	5.1760D 06	6.5250D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3590D 06	1.9000D 12
1.20	6.9730D 08	6.5890D 09	5.8070D 06	6.4340D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3430D 06	1.9000D 12
1.40	6.9680D 08	6.6040D 09	6.4370D 06	6.3440D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3330D 06	1.9000D 12
1.60	6.9630D 08	6.6180D 09	7.0660D 06	6.2550D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3280D 06	1.9000D 12
1.80	6.9590D 08	6.6320D 09	7.6930D 06	6.1680D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3270D 06	1.9000D 12
2.00	6.9540D 08	6.6460D 09	8.3190D 06	6.0820D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3310D 06	1.9000D 12
2.20	6.9500D 08	6.6600D 09	8.9440D 06	5.9970D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3390D 06	1.9000D 12
2.40	6.9450D 08	6.6740D 09	9.5680D 06	5.9130D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3510D 06	1.9000D 12
2.60	6.9410D 08	6.6870D 09	1.0190D 07	5.8300D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3680D 06	1.9000D 12
2.80	6.9360D 08	6.7010D 09	1.0810D 07	5.7480D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.3870D 06	1.9000D 12
3.00	6.9320D 08	6.7140D 09	1.1430D 07	5.6680D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4110D 06	1.9000D 12
3.20	6.9270D 08	6.7270D 09	1.2050D 07	5.5890D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4370D 06	1.9000D 12
3.40	6.9230D 08	6.7410D 09	1.2670D 07	5.5100D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.4670D 06	1.9000D 12
3.60	6.9180D 08	6.7540D 09	1.3290D 07	5.4330D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.5000D 06	1.9000D 12
3.80	6.9140D 08	6.7670D 09	1.3910D 07	5.3570D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.5350D 06	1.9000D 12
4.00	6.9090D 08	6.7790D 09	1.4520D 07	5.2820D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.5730D 06	1.9000D 12
4.20	6.9050D 08	6.7920D 09	1.5140D 07	5.2080D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.6140D 06	1.9000D 12
4.40	6.9000D 08	6.8050D 09	1.5750D 07	5.1350D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.6570D 06	1.9000D 12
4.60	6.8960D 08	6.8170D 09	1.6370D 07	5.0630D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.7020D 06	1.9000D 12
4.80	6.8910D 08	6.8300D 09	1.6980D 07	4.9920D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.7500D 06	1.9000D 12
5.00	6.8870D 08	6.8420D 09	1.7590D 07	4.9220D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.7990D 06	1.9000D 12
5.20	6.8820D 08	6.8540D 09	1.8210D 07	4.8530D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.8510D 06	1.9000D 12
5.40	6.8780D 08	6.8660D 09	1.8820D 07	4.7850D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.9040D 06	1.9000D 12
5.60	6.8730D 08	6.8780D 09	1.9430D 07	4.7180D 08	4.2000D 12	1.7000D 17	2.0000D 09	1.9590D 06	1.9000D 12
5.80	6.8690D 08	6.8900D 09	2.0040D 07	4.6520D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.0150D 06	1.9000D 12
6.00	6.8640D 08	6.9020D 09	2.0650D 07	4.5870D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.0740D 06	1.9000D 12
6.20	6.8600D 08	6.9130D 09	2.1260D 07	4.5220D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.1330D 06	1.9000D 12
6.40	6.8550D 08	6.9250D 09	2.1860D 07	4.4590D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.1940D 06	1.9000D 12
6.60	6.8510D 08	6.9360D 09	2.2470D 07	4.3960D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.2560D 06	1.9000D 12
6.80	6.8460D 08	6.9480D 09	2.3080D 07	4.3350D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.3200D 06	1.9000D 12
7.00	6.8420D 08	6.9590D 09	2.3690D 07	4.2740D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.3840D 06	1.9000D 12
7.20	6.8370D 08	6.9700D 09	2.4290D 07	4.2140D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.4500D 06	1.9000D 12
7.40	6.8330D 08	6.9810D 09	2.4900D 07	4.1540D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.5160D 06	1.9000D 12
7.60	6.8280D 08	6.9920D 09	2.5500D 07	4.0960D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.5840D 06	1.9000D 12
7.80	6.8240D 08	7.0030D 09	2.6110D 07	4.0390D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.6520D 06	1.9000D 12
8.00	6.8200D 08	7.0140D 09	2.6710D 07	3.9820D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.7210D 06	1.9000D 12
8.20	6.8150D 08	7.0250D 09	2.7320D 07	3.9260D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.7910D 06	1.9000D 12
8.40	6.8110D 08	7.0350D 09	2.7920D 07	3.8710D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.8620D 06	1.9000D 12
8.60	6.8060D 08	7.0460D 09	2.8520D 07	3.8160D 08	4.2000D 12	1.7000D 17	2.0000D 09	2.9330D 06	1.9000D 12
8.80	6.8020D 08	7.0560D 09	2.9130D 07	3.7620D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.0050D 06	1.9000D 12
9.00	6.7970D 08	7.0670D 09	2.9730D 07	3.7090D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.0780D 06	1.9000D 12
9.20	6.7930D 08	7.0770D 09	3.0330D 07	3.6570D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.1510D 06	1.9000D 12
9.40	6.7890D 08	7.0870D 09	3.0940D 07	3.6060D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.2250D 06	1.9000D 12
9.60	6.7840D 08	7.0970D 09	3.1540D 07	3.5550D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.2990D 06	1.9000D 12
9.80	6.7800D 08	7.1080D 09	3.2140D 07	3.5050D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.3730D 06	1.9000D 12
10.00	6.7750D 08	7.1180D 09	3.2740D 07	3.4560D 08	4.2000D 12	1.7000D 17	2.0000D 09	3.4480D 06	1.9000D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.3000D 07	1.8000D 09	1.0000D 06	8.0000D 05	3.5000D 09	4.0000D 08
0.20	2.0590D 02	7.70[illegible]D-06	1.0000D 06	2.9160D 07	1.8000D 09	1.0000D 06	8.0020D 05	3.4950D 09	4.0000D 08
0.40	1.9810D 02	7.3120D-06	1.0000D 06	3.4330D 07	1.8000D 09	1.0000D 06	8.0040D 05	3.4900D 09	3.9990D 08
0.60	1.9810D 02	7.1430D-06	1.0000D 06	3.9490D 07	1.8000D 09	1.0000D 06	8.0060D 05	3.4850D 09	3.9990D 08
0.80	1.9810D 02	7.0060D-06	1.0000D 06	4.4640D 07	1.8000D 09	1.0000D 06	8.0070D 05	3.4790D 09	3.9990D 08
1.00	1.9810D 02	6.8990D-06	1.0000D 06	4.9760D 07	1.8000D 09	1.0000D 06	8.0090D 05	3.4740D 09	3.9980D 08
1.20	1.9810D 02	6.8200D-06	1.0000D 06	5.4880D 07	1.8000D 09	1.0000D 06	8.0110D 05	3.4690D 09	3.9980D 08
1.40	1.9810D 02	6.7670D-06	1.0000D 06	5.9980D 07	1.8000D 09	1.0000D 06	8.0120D 05	3.4640D 09	3.9980D 08
1.60	1.9810D 02	6.7400D-06	1.0000D 06	6.5060D 07	1.8000D 09	1.0000D 06	8.0140D 05	3.4590D 09	3.9970D 08
1.80	1.9810D 02	6.7370D-06	1.0000D 06	7.0140D 07	1.8000D 09	1.0000D 06	8.0150D 05	3.4540D 09	3.9970D 08
2.00	1.9810D 02	6.7560D-06	1.0000D 06	7.5190D 07	1.8000D 09	1.0000D 06	8.0170D 05	3.4490D 09	3.9970D 08
2.20	1.9810D 02	6.7980D-06	1.0000D 06	8.0240D 07	1.8000D 09	1.0000D 06	8.0180D 05	3.4440D 09	3.9960D 08
2.40	1.9810D 02	6.8600D-06	1.0000D 06	8.5270D 07	1.8000D 09	1.0000D 06	8.0200D 05	3.4390D 09	3.9960D 08
2.60	1.9810D 02	6.9420D-06	1.0000D 06	9.0290D 07	1.8000D 09	1.0000D 06	8.0210D 05	3.4340D 09	3.9960D 08
2.80	1.9810D 02	7.0420D-06	1.0000D 06	9.5300D 07	1.8000D 09	1.0000D 06	8.0230D 05	3.4290D 09	3.9950D 08
3.00	1.9810D 02	7.1600D-06	1.0000D 06	1.0030D 08	1.8000D 09	1.0000D 06	8.0240D 05	3.4240D 09	3.9950D 08
3.20	1.9810D 02	7.2950D-06	1.0000D 06	1.0530D 08	1.8000D 09	1.0000D 06	8.0250D 05	3.4190D 09	3.9950D 08
3.40	1.9810D 02	7.4460D-06	1.0000D 06	1.1020D 08	1.8000D 09	1.0000D 06	8.0270D 05	3.4140D 09	3.9950D 08
3.60	1.9810D 02	7.6120D-06	1.0000D 06	1.1520D 08	1.8000D 09	1.0000D 06	8.0280D 05	3.4090D 09	3.9940D 08
3.80	1.9810D 02	7.7920D-06	1.0000D 06	1.2010D 08	1.8000D 09	1.0000D 06	8.0300D 05	3.4040D 09	3.9940D 08
4.00	1.9810D 02	7.9860D-06	1.0000D 06	1.2510D 08	1.8000D 09	1.0000D 06	8.0310D 05	3.3990D 09	3.9940D 08
4.20	1.9810D 02	8.1920D-06	1.0000D 06	1.3000D 08	1.8000D 09	1.0000D 06	8.0330D 05	3.3940D 09	3.9930D 08
4.40	1.9810D 02	8.4110D-06	1.0000D 06	1.3490D 08	1.8000D 09	1.0000D 06	8.0350D 05	3.3890D 09	3.9930D 08
4.60	1.9810D 02	8.6410D-06	1.0000D 06	1.3980D 08	1.8000D 09	1.0000D 06	8.0360D 05	3.3840D 09	3.9930D 08
4.80	1.9810D 02	8.8820D-06	1.0000D 06	1.4470D 08	1.8000D 09	1.0000D 06	8.0380D 05	3.3790D 09	3.9920D 08
5.00	1.9810D 02	9.1340D-06	1.0000D 06	1.4950D 08	1.8000D 09	1.0000D 06	8.0390D 05	3.3740D 09	3.9920D 08
5.20	1.9810D 02	9.3950D-06	1.0000D 06	1.5440D 08	1.8000D 09	1.0000D 06	8.0410D 05	3.3690D 09	3.9920D 08
5.40	1.9810D 02	9.6660D-06	1.0000D 06	1.5920D 08	1.8000D 09	1.0000D 06	8.0430D 05	3.3640D 09	3.9910D 08
5.60	1.9320D 02	9.9450D-06	1.0000D 06	1.6410D 08	1.8000D 09	1.0000D 06	8.0440D 05	3.3590D 09	3.9910D 08
5.80	1.9820D 02	1.0230D-05	1.0000D 06	1.6890D 08	1.8000D 09	1.0000D 06	8.0460D 05	3.3540D 09	3.9910D 08
6.00	1.9820D 02	1.0530D-05	1.0000D 06	1.7370D 08	1.8000D 09	1.0000D 06	8.0480D 05	3.3490D 09	3.9900D 08
6.20	1.9820D 02	1.0830D-05	1.0000D 06	1.7850D 08	1.8000D 09	1.0000D 06	8.0500D 05	3.3440D 09	3.9900D 08
6.40	1.9820D 02	1.1140D-05	1.0000D 06	1.8330D 08	1.8000D 09	1.0000D 06	8.0510D 05	3.3390D 09	3.9900D 08
6.60	1.9820D 02	1.1460D-05	1.0000D 06	1.8810D 08	1.8000D 09	1.0000D 06	8.0530D 05	3.3340D 09	3.9890D 08
6.80	1.9820D 02	1.1780D-05	1.0000D 06	1.9280D 08	1.8000D 09	1.0000D 06	8.0550D 05	3.3300D 09	3.9890D 08
7.00	1.9820D 02	1.2100D-05	1.0000D 06	1.9760D 08	1.8000D 09	1.0000D 06	8.0570D 05	3.3250D 09	3.9890D 08
7.20	1.9820D 02	1.2440D-05	1.0000D 06	2.0230D 08	1.8000D 09	1.0000D 06	8.0590D 05	3.3200D 09	3.9880D 08
7.40	1.9820D 02	1.2780D-05	1.0000D 06	2.0710D 08	1.8000D 09	1.0000D 06	8.0610D 05	3.3150D 09	3.9880D 08
7.60	1.9820D 02	1.3120D-05	1.0000D 06	2.1180D 08	1.8000D 09	1.0000D 06	8.0630D 05	3.3100D 09	3.9880D 08
7.80	1.9820D 02	1.3470D-05	1.0000D 06	2.1650D 08	1.8000D 09	1.0000D 06	8.0650D 05	3.3050D 09	3.9880D 08
8.00	1.9820D 02	1.3820D-05	1.0000D 06	2.2120D 08	1.8000D 09	1.0000D 06	8.0670D 05	3.3000D 09	3.9870D 08
8.20	1.9820D 02	1.4180D-05	1.0000D 06	2.2590D 08	1.8000D 09	1.0000D 06	8.0690D 05	3.2960D 09	3.9870D 08
8.40	1.9830D 02	1.4530D-05	1.0000D 06	2.3050D 08	1.8010D 09	1.0000D 06	8.0710D 05	3.2910D 09	3.9870D 08
8.60	1.9830D 02	1.4900D-05	1.0000D 06	2.3520D 08	1.8010D 09	1.0000D 06	8.0730D 05	3.2860D 09	3.9860D 08
8.80	1.9830D 02	1.5260D-05	1.0000D 06	2.3990D 08	1.8010D 09	1.0000D 06	8.0750D 05	3.2810D 09	3.9860D 08
9.00	1.9830D 02	1.5630D-05	1.0000D 06	2.4450D 08	1.8010D 09	1.0000D 06	8.0770D 05	3.2760D 09	3.9860D 08
9.20	1.9830D 02	1.6000D-05	1.0000D 06	2.4910D 08	1.8010D 09	1.0000D 06	8.0790D 05	3.2720D 09	3.9850D 08
9.40	1.9830D 02	1.6380D-05	1.0000D 06	2.5370D 08	1.8010D 09	1.0000D 06	8.0810D 05	3.2670D 09	3.9850D 08
9.60	1.9830D 02	1.6760D-05	1.0000D 06	2.5830D 08	1.8010D 09	1.0000D 06	8.0830D 05	3.2620D 09	3.9850D 08
9.80	1.9830D 02	1.7140D-05	1.0000D 06	2.6290D 08	1.8010D 09	1.0000D 06	8.0850D 05	3.2570D 09	3.9840D 08
10.00	1.9840D 02	1.7520D-05	1.0000D 06	2.6750D 08	1.8010D 09	1.0000D 06	8.0880D 05	3.2530D 09	3.9840D 08

T= 700 K, H= 25 km, 19 torr

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	4.80D 05	4.94D-15
2	2*NO3 >>> 2*NO2 + O2	2.57D-14	7.44D-49
3	NO2 + NO3 >>> NO2 + NO + O2	5.51D-14	3.97D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.23D-1?
5	NO + O3 >>> NO2 + O2	2.65D-13	4.54D-28
6	NO2 + O3 >>> NO3 + O2	3.62D-15	6.56D-22
7	HNO3 + M >>> HO + NO2 + M	4.01D-02	6.70D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	4.74D-19
9	O + O + M >>> O2 + M	9.50D-17	6.21D-21
10	O + O2 + M >>> O3 + M	5.55D-17	3.36D 00
11	O + O3 >>> 2*O2	7.11D-13	8.63D-43
12	O + NO + M >>> NO2 + M	9.01D-15	2.14D-11
13	O + NO2 >>> NO + O2	1.11D-11	8.50D-27
14	O + NO2 + M >>> NO3 + M	2.53D-14	2.02D-24
15	HO + HO >>> H2O + O	4.53D-12	2.04D-16
16	O2 + 2*NO >>> 2*NO2	7.04D-39	9.37D-21
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.11D-15
19	O + HO2 >>> HO + O2	3.91D-11	2.19D-28
20	O2 + H + M >>> HO2 + M	2.75D-15	6.18D-06
21	O3 + H >>> HO + O2	4.78D-11	5.62D-37
22	O3 + HO >>> HO2 + O2	3.59D-13	8.31D-26
23	O3 + HO2 >>> HO + 2*O2	1.18D-14	1.12D-49
24	H + HO + M >>> H2O + M	1.39D-14	3.35D-27
25	H + HO2 >>> 2*HO	1.08D-10	5.87D-24
26	H + HO2 >>> H2 + O2	2.55D-11	8.03D-26
27	H + H2O >>> H2 + HO	6.56D-17	8.90D-13
28	H + H2O2 >>> H2 + HO2	3.06D-13	1.77D-19
29	H + H2O2 >>> HO + H2O	3.98D-13	1.02D-35

30	2*HO + M >>> H2O2 + M	1.14D-14	1.04D-04
31	HO + HO2 >>> H2O + O2	4.06D-11	7.73D-33
32	2*HO2 >>> H2O2 + O2	4.32D-12	3.02D-24
33	HO2 + H2O >>> H2O2 + HO	2.72D-21	3.07D-12
34	NO + H + M >>> HNO + M	2.91D-15	2.20D-06
35	NO + HO >>> HO2 + H	2.23D-21	2.02D-10
36	NO + HO + M >>> HNO2 + M	4.76D-14	5.93D-03
37	NO + HO2 >>> NO2 + HO	3.60D-12	2.68D-14
38	H + H + M >>> H2 + M	2.53D-16	2.11D-25
39	HNO4 + M >>> HO2 + NO2 + M	6.57D 05	6.14D-15
40	CLNO3 + M >>> CLO + NO2 + M	3.75D 05	2.59D-15

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	7.000D 08	6.500D 09	2.000D 06	7.000D 08	4.200D 12	1.700D 17	2.000D 09	1.500D 06	1.900D 12
0.20	2.508D-02	3.358D 09	7.268D 08	8.433D 09	2.417D 12	1.700D 17	1.984D 09	2.264D 09	1.900D 12
0.40	9.278D-03	1.268D 09	7.117D 08	1.055D 10	2.300D 12	1.700D 17	1.968D 09	2.304D 09	1.900D 12
0.60	6.694D-03	9.461D 08	6.884D 08	1.091D 10	1.961D 12	1.700D 17	1.953D 09	2.334D 09	1.900D 12
0.80	6.051D-03	8.864D 08	6.642D 08	1.101D 10	1.707D 12	1.700D 17	1.937D 09	2.355D 09	1.900D 12
1.00	5.755D-03	8.745D 08	6.403D 08	1.106D 10	1.510D 12	1.700D 17	1.921D 09	2.370D 09	1.900D 12
1.20	5.538D-03	8.735D 08	6.168D 08	1.110D 10	1.352D 12	1.700D 17	1.906D 09	2.379D 09	1.900D 12
1.40	5.347D-03	8.758D 08	5.940D 08	1.114D 10	1.223D 12	1.700D 17	1.891D 09	2.384D 09	1.900D 12
1.60	5.168D-03	8.792D 08	5.719D 08	1.117D 10	1.116D 12	1.700D 17	1.876D 09	2.385D 09	1.900D 12
1.80	4.996D-03	8.832D 08	5.503D 08	1.121D 10	1.025D 12	1.700D 17	1.861D 09	2.384D 09	1.900D 12
2.00	4.830D-03	8.875D 08	5.295D 08	1.124D 10	9.469D 11	1.700D 17	1.846D 09	2.379D 09	1.900D 12
2.20	4.668D-03	8.918D 08	5.093D 08	1.127D 10	8.796D 11	1.700D 17	1.831D 09	2.373D 09	1.900D 12
2.40	4.512D-03	8.962D 08	4.898D 08	1.130D 10	8.207D 11	1.700D 17	1.816D 09	2.365D 09	1.900D 12
2.60	4.359D-03	9.006D 08	4.710D 08	1.133D 10	7.689D 11	1.700D 17	1.802D 09	2.355D 09	1.900D 12
2.80	4.211D-03	9.049D 08	4.528D 08	1.135D 10	7.229D 11	1.700D 17	1.787D 09	2.345D 09	1.900D 12
3.00	4.067D-03	9.092D 08	4.352D 08	1.138D 10	6.819D 11	1.700D 17	1.773D 09	2.333D 09	1.900D 12
3.20	3.927D-03	9.134D 08	4.183D 08	1.141D 10	6.450D 11	1.700D 17	1.759D 09	2.320D 09	1.900D 12
3.40	3.790D-03	9.175D 08	4.020D 08	1.143D 10	6.116D 11	1.700D 17	1.745D 09	2.307D 09	1.900D 12
3.60	3.658D-03	9.214D 08	3.862D 08	1.146D 10	5.814D 11	1.700D 17	1.731D 09	2.293D 09	1.900D 12
3.80	3.529D-03	9.253D 08	3.711D 08	1.148D 10	5.538D 11	1.700D 17	1.717D 09	2.279D 09	1.900D 12
4.00	3.404D-03	9.290D 08	3.565D 08	1.151D 10	5.285D 11	1.700D 17	1.703D 09	2.264D 09	1.900D 12
4.20	3.282D-03	9.327D 08	3.424D 08	1.153D 10	5.054D 11	1.700D 17	1.690D 09	2.249D 09	1.900D 12
4.40	3.164D-03	9.362D 08	3.289D 08	1.156D 10	4.840D 11	1.700D 17	1.676D 09	2.234D 09	1.900D 12
4.60	3.050D-03	9.396D 08	3.159D 08	1.158D 10	4.643D 11	1.700D 17	1.663D 09	2.218D 09	1.900D 12
4.80	2.939D-03	9.429D 08	3.033D 08	1.160D 10	4.459D 11	1.700D 17	1.649D 09	2.203D 09	1.900D 12
5.00	2.832D-03	9.461D 08	2.913D 08	1.162D 10	4.289D 11	1.700D 17	1.636D 09	2.187D 09	1.900D 12
5.20	2.728D-03	9.491D 08	2.797D 08	1.164D 10	4.131D 11	1.700D 17	1.623D 09	2.172D 09	1.900D 12
5.40	2.628D-03	9.521D 08	2.686D 08	1.166D 10	3.983D 11	1.700D 17	1.610D 09	2.156D 09	1.900D 12
5.60	2.531D-03	9.550D 08	2.579D 08	1.169D 10	3.844D 11	1.700D 17	1.597D 09	2.140D 09	1.900D 12
5.80	2.437D-03	9.577D 08	2.476D 08	1.171D 10	3.714D 11	1.700D 17	1.584D 09	2.124D 09	1.900D 12
6.00	2.346D-03	9.604D 08	2.377D 08	1.173D 10	3.592D 11	1.700D 17	1.572D 09	2.109D 09	1.900D 12
6.20	2.258D-03	9.630D 08	2.282D 08	1.174D 10	3.477D 11	1.700D 17	1.559D 09	2.093D 09	1.900D 12
6.40	2.174D-03	9.655D 08	2.191D 08	1.176D 10	3.369D 11	1.700D 17	1.547D 09	2.078D 09	1.900D 12
6.60	2.092D-03	9.679D 08	2.103D 08	1.178D 10	3.266D 11	1.700D 17	1.534D 09	2.062D 09	1.900D 12
6.80	2.013D-03	9.702D 08	2.019D 08	1.180D 10	3.170D 11	1.700D 17	1.522D 09	2.047D 09	1.900D 12
7.00	1.937D-03	9.725D 08	1.938D 08	1.182D 10	3.078D 11	1.700D 17	1.510D 09	2.032D 09	1.900D 12
7.20	1.864D-03	9.747D 08	1.861D 08	1.184D 10	2.991D 11	1.700D 17	1.498D 09	2.017D 09	1.900D 12
7.40	1.793D-03	9.768D 08	1.786D 08	1.185D 10	2.908D 11	1.700D 17	1.486D 09	2.002D 09	1.900D 12
7.60	1.725D-03	9.788D 08	1.715D 08	1.187D 10	2.830D 11	1.700D 17	1.474D 09	1.988D 09	1.900D 12
7.80	1.659D-03	9.808D 08	1.646D 08	1.189D 10	2.755D 11	1.700D 17	1.462D 09	1.973D 09	1.900D 12
8.00	1.596D-03	9.827D 08	1.580D 08	1.190D 10	2.684D 11	1.700D 17	1.451D 09	1.959D 09	1.900D 12
8.20	1.535D-03	9.846D 08	1.517D 08	1.192D 10	2.616D 11	1.700D 17	1.439D 09	1.945D 09	1.900D 12
8.40	1.476D-03	9.864D 08	1.456D 08	1.193D 10	2.551D 11	1.700D 17	1.427D 09	1.931D 09	1.900D 12
8.60	1.420D-03	9.881D 08	1.398D 08	1.195D 10	2.489D 11	1.700D 17	1.416D 09	1.917D 09	1.901D 12
8.80	1.366D-03	9.898D 08	1.342D 08	1.196D 10	2.430D 11	1.700D 17	1.405D 09	1.903D 09	1.901D 12
9.00	1.313D-03	9.915D 08	1.289D 08	1.198D 10	2.373D 11	1.700D 17	1.393D 09	1.890D 09	1.901D 12
9.20	1.263D-03	9.931D 08	1.237D 08	1.199D 10	2.318D 11	1.700D 17	1.382D 09	1.876D 09	1.901D 12
9.40	1.215D-03	9.947D 08	1.188D 08	1.201D 10	2.266D 11	1.700D 17	1.371D 09	1.863D 09	1.901D 12
9.60	1.168D-03	9.962D 08	1.141D 08	1.202D 10	2.216D 11	1.700D 17	1.360D 09	1.850D 09	1.901D 12
9.80	1.124D-03	9.977D 08	1.096D 08	1.203D 10	2.167D 11	1.700D 17	1.349D 09	1.837D 09	1.901D 12
10.00	1.081D-03	9.992D 08	1.052D 08	1.205D 10	2.121D 11	1.700D 17	1.339D 09	1.825D 09	1.901D 12

TIME(S)	O	H	HO	HO2	H2O2	H2O	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.3000D 07	1.8000D 09	1.0000D 06	8.0000D 05	3.5000D 09	4.0000D 08
0.20	8.0540D 11	7.9630D 07	1.3670D 06	1.2430D 09	1.8040D 09	1.0000D 06	6.8880D 05	3.9000D-02	1.059D-02
0.40	7.3500D 11	7.5990D 07	1.8850D 06	1.2860D 09	1.8050D 09	1.001D 06	1.101D 06	1.525D-02	4.000D-03
0.60	6.4020D 11	6.8220D 07	2.3730D 06	1.3230D 09	1.8050D 09	1.0010D 06	1.3380D 06	1.170D-02	2.984D-03
0.80	5.6370D 11	6.1430D 07	2.4220D 06	1.3510D 09	1.8050D 09	1.0010D 06	1.5810D 06	1.120D-02	2.796D-03
1.00	5.0260D 11	5.5690D 07	3.2340D 06	1.3720D 09	1.8060D 09	1.0020D 06	1.8270D 06	1.122D-02	2.758D-03
1.20	4.5290D 11	5.0800D 07	3.6140D 06	1.3880D 09	1.8060D 09	1.0020D 06	2.0750D 06	1.133D-02	2.755D-03
1.40	4.1170D 11	4.6600D 07	3.9650D 06	1.3990D 09	1.8070D 09	1.0030D 06	2.3250D 06	1.146D-02	2.762D-03
1.60	3.7710D 11	4.2960D 07	4.2890D 06	1.4070D 09	1.8070D 09	1.0030D 06	2.5750D 06	1.157D-02	2.773D-03
1.80	3.4770D 11	3.9770D 07	4.5890D 06	1.4120D 09	1.8080D 09	1.0030D 06	2.8260D 06	1.166D-02	2.786D-03
2.00	3.2220D 11	3.6950D 07	4.8690D 06	1.4150D 09	1.8080D 09	1.0030D 06	3.0770D 06	1.174D-02	2.799D-03
2.20	3.0010D 11	3.4450D 07	5.1290D 06	1.4150D 09	1.8090D 09	1.0040D 06	3.3280D 06	1.180D-02	2.813D-03
2.40	2.8070D 11	3.2210D 07	5.3710D 06	1.4140D 09	1.8100D 09	1.0040D 06	3.5780D 06	1.185D-02	2.826D-03
2.60	2.6350D 11	3.0200D 07	5.5980D 06	1.4120D 09	1.8100D 09	1.0040D 06	3.8280D 06	1.188D-02	2.840D-03
2.80	2.4820D 11	2.8390D 07	5.8090D 06	1.4080D 09	1.8110D 09	1.0040D 06	4.0770D 06	1.191D-02	2.854D-03
3.00	2.3440D 11	2.6750D 07	6.0080D 06	1.4030D 09	1.8120D 09	1.0040D 06	4.3250D 06	1.193D-02	2.867D-03
3.20	2.2210D 11	2.5250D 07	6.1950D 06	1.3980D 09	1.8120D 09	1.0050D 06	4.572D 06	1.194D-02	2.881D-03
3.40	2.1090D 11	2.3880D 07	6.3700D 06	1.3920D 09	1.8130D 09	1.0050D 06	4.818D 06	1.194D-02	2.893D-03
3.60	2.0070D 11	2.2630D 07	6.5350D 06	1.3850D 09	1.8140D 09	1.0050D 06	5.063D 06	1.193D-02	2.906D-03
3.80	1.9140D 11	2.1480D 07	6.6900D 06	1.3780D 09	1.8140D 09	1.0050D 06	5.306D 06	1.192D-02	2.918D-03
4.00	1.8280D 11	2.0420D 07	6.8370D 06	1.3700D 09	1.8150D 09	1.005D 06	5.549D 06	1.190D-02	2.930D-03
4.20	1.7500D 11	1.9430D 07	6.9760D 06	1.3620D 09	1.8150D 09	1.005D 06	5.789D 06	1.187D-02	2.941D-03
4.40	1.6770D 11	1.8520D 07	7.1070D 06	1.3540D 09	1.8160D 09	1.005D 06	6.029D 06	1.185D-02	2.953D-03
4.60	1.6100D 11	1.7680D 07	7.2310D 06	1.3450D 09	1.8160D 09	1.006D 06	6.267D 06	1.181D-02	2.963D-03
4.80	1.5480D 11	1.6890D 07	7.3480D 06	1.3360D 09	1.8170D 09	1.006D 06	6.503D 06	1.178D-02	2.974D-03
5.00	1.4900D 11	1.6160D 07	7.4600D 06	1.3270D 09	1.8170D 09	1.006D 06	6.738D 06	1.174D-02	2.984D-03
5.20	1.4350D 11	1.5470D 07	7.5650D 06	1.3180D 09	1.8180D 09	1.006D 06	6.971D 06	1.170D-02	2.993D-03
5.40	1.3950D 11	1.4830D 07	7.6660D 06	1.3090D 09	1.8180D 09	1.006D 06	7.202D 06	1.165D-02	3.003D-03
5.60	1.3370D 11	1.4230D 07	7.7610D 06	1.3000D 09	1.8190D 09	1.006D 06	7.432D 06	1.160D-02	3.012D-03
5.80	1.2930D 11	1.3670D 07	7.8520D 06	1.2910D 09	1.8190D 09	1.006D 06	7.661D 06	1.155D-02	3.021D-03
6.00	1.2510D 11	1.3130D 07	7.9390D 06	1.2810D 09	1.8190D 09	1.006D 06	7.888D 06	1.150D-02	3.029D-03
6.20	1.2120D 11	1.2640D 07	8.0220D 06	1.2720D 09	1.8200D 09	1.006D 06	8.113D 06	1.145D-02	3.037D-03
6.40	1.1740D 11	1.2160D 07	8.1000D 06	1.2630D 09	1.8200D 09	1.006D 06	8.337D 06	1.140D-02	3.045D-03
6.60	1.1390D 11	1.1720D 07	8.1750D 06	1.2530D 09	1.8200D 09	1.006D 06	8.558D 06	1.134D-02	3.053D-03
6.80	1.1060D 11	1.1300D 07	8.2470D 06	1.2440D 09	1.8210D 09	1.007D 06	8.779D 06	1.128D-02	3.060D-03
7.00	1.0740D 11	1.0900D 07	8.3160D 06	1.2350D 09	1.8210D 09	1.007D 06	8.998D 06	1.123D-02	3.067D-03
7.20	1.0440D 11	1.0520D 07	8.3810D 06	1.2260D 09	1.8210D 09	1.007D 06	9.215D 06	1.117D-02	3.074D-03
7.40	1.0160D 11	1.0170D 07	8.4440D 06	1.2170D 09	1.8210D 09	1.007D 06	9.430D 06	1.111D-02	3.081D-03
7.60	9.8870D 10	9.8270D 06	8.5040D 06	1.2080D 09	1.8210D 09	1.007D 06	9.644D 06	1.105D-02	3.087D-03
7.80	9.6290D 10	9.5050D 06	8.5620D 06	1.1990D 09	1.8220D 09	1.007D 06	9.856D 06	1.099D-02	3.093D-03
8.00	9.3830D 10	9.1990D 06	8.6170D 06	1.1900D 09	1.8220D 09	1.007D 06	1.007D 07	1.093D-02	3.099D-03
8.20	9.1480D 10	8.9070D 06	8.6700D 06	1.1810D 09	1.8220D 09	1.007D 06	1.028D 07	1.087D-02	3.105D-03
8.40	8.9240D 10	8.6290D 06	8.7210D 06	1.1730D 09	1.8220D 09	1.007D 06	1.048D 07	1.081D-02	3.111D-03
8.60	8.7090D 10	8.3640D 06	8.7690D 06	1.1640D 09	1.8220D 09	1.007D 06	1.069D 07	1.075D-02	3.116D-03
8.80	8.5040D 10	8.1110D 06	8.8160D 06	1.1560D 09	1.8220D 09	1.007D 06	1.089D 07	1.069D-02	3.122D-03
9.00	8.3070D 10	7.8700D 06	8.8610D 06	1.1470D 09	1.8220D 09	1.007D 06	1.110D 07	1.063D-02	3.127D-03
9.20	8.1180D 10	7.6390D 06	8.9040D 06	1.1390D 09	1.8220D 09	1.007D 06	1.130D 07	1.057D-02	3.132D-03
9.40	7.9370D 10	7.4180D 06	8.9460D 06	1.1310D 09	1.8220D 09	1.007D 06	1.150D 07	1.051D-02	3.137D-03
9.60	7.7630D 10	7.2070D 06	8.9860D 06	1.1220D 09	1.8220D 09	1.007D 06	1.170D 07	1.045D-02	3.142D-03
9.80	7.5960D 10	7.005D 06	9.0250D 06	1.114D 09	1.822D 09	1.007D 06	1.190D 07	1.039D-02	3.147D-03
10.00	7.435D 10	6.811D 06	9.062D 06	1.106D 09	1.822D 09	1.008D 06	1.209D 07	1.033D-02	3.151D-03

T=800 K, H= 25 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	2.65D 00	3.70D-15
2	2*NO3 >>> 2*NO2 + O2	3.98D-14	5.95D-48
3	NO2 + NO3 >>> NO2 + NO + O2	6.59D-14	3.13D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.74D-18
5	NO + O3 >>> NO2 + O2	3.43D-13	4.42D-26
6	NO2 + O3 >>> NO3 + O2	5.61D-15	9.78D-21
7	HNO3 + M >>> HO + NO2 + M	1.90D 00	4.20D-14
8	HNO3 + HO >>> H2O + NO3	[illegible].00D-14	2.43D-18
9	O + O + M >>> O2 + M	7.08D-17	1.87D-16
10	O + O2 + M >>> O3 + M	4.43D-17	2.26D 01
11	O + O3 >>> 2*O2	1.07D-12	6.11D-39
12	O + NO + M >>> NO2 + M	7.11D-15	6.78D-09
13	O + NO2 >>> NO + O2	1.17D-11	5.55D-25
14	O + NO2 + M >>> NO3 + M	2.21D-14	1.77D-24
15	HO + HO >>> H2O + O	5.00D-12	1.06D-15
16	O2 + 2*NO >>> 2*NO2	6.40D-39	8.78D-20
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	9.55D-15
19	O + HO2 >>> HO + O2	4.28D-11	3.43D-26
20	O2 + H + M >>> HO2 + M	2.20D-15	3.28D-04
21	O3 + H >>> HO + O2	5.25D-11	6.31D-34
22	O3 + HO >>> HO2 + O2	4.30D-13	3.24D-24
23	O3 + HO2 >>> HO + 2*O2	1.48D-14	2.35D-49
24	H + HO + M >>> H2O + M	8.61D-15	8.52D-23
25	H + HO2 >>> 2*HO	1.28D-10	2.16D-22
26	H + HO2 >>> H2 + O2	2.71D-11	1.45D-26
27	H + H2O >>> H2 + HO	4.09D-16	1.41D-12
28	H + H2O2 >>> H2 + HO2	3.93D-13	9.47D-18
29	H + H2O2 >>> HO + H2O	5.11D-13	6.02D-33

30	2*HO + M >>> H2O2 + M	8.50D-15	7.01D-03
31	HO + HO2 >>> H2O + O2	4.44D-11	5.70D-30
32	2*HO2 >>> H2O2 + O2	3.10D-12	1.53D-22
33	HO2 + H2O >>> H2O2 + HO	5.19D-20	3.46D-12
34	NO + H + M >>> HNO + M	2.41D-15	1.43D-04
35	NO + HO >>> NO2 + H	3.30D-20	2.30D-10
36	NO + HO + M >>> HNO2 + M	3.42D-14	3.25D-01
37	NO + HO2 >>> NO2 + HO	4.46D-12	7.66D-14
38	H + H + M >>> H2 + M	2.21D-15	2.33D-21
39	HNO4 + M >>> HO2 + NO2 + M	3.48D 06	4.55D-15
40	CLNO3 + M >>> CLO + NO2 + M	2.43D 06	1.50D-15

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	7.000D 08	6.500D 09	2.000D 06	7.000D 08	4.200D 12	1.700D 17	2.000D 09	1.500D 06	1.900D 12
0.20	2.950D-04	2.983D 08	7.082D 08	1.213D 10	7.378D 11	1.700D 17	1.368D 09	4.771D 09	1.899D 12
0.40	2.153D-04	2.275D 08	6.777D 08	1.266D 10	5.876D 11	1.700D 17	9.360D 08	6.384D 09	1.898D 12
0.60	2.009D-04	2.223D 08	6.471D 08	1.299D 10	4.680D 11	1.700D 17	6.403D 08	7.552D 09	1.898D 12
0.80	1.868D-04	2.169D 08	6.169D 08	1.323D 10	4.151D 11	1.700D 17	4.380D 08	8.391D 09	1.898D 12
1.00	1.738D-04	2.118D 08	5.875D 08	1.340D 10	3.594D 11	1.700D 17	2.996D 08	8.987D 09	1.897D 12
1.20	1.621D-04	2.076D 08	5.590D 08	1.353D 10	3.156D 11	1.700D 17	2.050D 08	9.400D 09	1.897D 12
1.40	1.518D-04	2.044D 08	5.316D 08	1.362D 10	2.604D 11	1.700D 17	1.402D 08	9.674D 09	1.897D 12
1.60	1.427D-04	2.023D 08	5.053D 08	1.369D 10	2.515D 11	1.700D 17	9.592D 07	9.843D 09	1.897D 12
1.80	1.349D-04	2.010D 08	4.802D 08	1.375D 10	2.274D 11	1.700D 17	6.563D 07	9.933D 09	1.897D 12
2.00	1.277D-04	2.004D 08	4.562D 08	1.380D 10	2.070D 11	1.700D 17	4.490D 07	9.962D 09	1.897D 12
2.20	1.213D-04	2.004D 08	4.333D 08	1.383D 10	1.896D 11	1.700D 17	3.073D 07	9.945D 09	1.897D 12
2.40	1.154D-04	2.00 D 08	4.114D 08	1.386D 10	1.745D 11	1.700D 17	2.103D 07	9.893D 09	1.897D 12
2.60	1.100D-04	2.017D 08	3.906D 08	1.389D 10	1.614D 11	1.700D 17	1.440D 07	9.814D 09	1.897D 12
2.80	1.050D-04	2.028D 08	3.709D 08	1.391D 10	1.499D 11	1.700D 17	9.866D 06	9.715D 09	1.897D 12
3.00	1.003D-04	2.040D 08	3.520D 08	1.393D 10	1.398D 11	1.700D 17	6.762D 06	9.602D 09	1.897D 12
3.20	9.581D-05	2.053D 08	3.342D 08	1.395D 10	1.307D 11	1.700D 17	4.640D 06	9.478D 09	1.897D 12
3.40	9.153D-05	2.067D 08	3.172D 08	1.397D 10	1.227D 11	1.700D 17	3.187D 06	9.347D 09	1.897D 12
3.60	8.743D-05	2.080D 08	3.010D 08	1.398D 10	1.154D 11	1.700D 17	2.194D 06	9.211D 09	1.897D 12
3.80	8.350D-05	2.093D 08	2.856D 08	1.400D 10	1.088D 11	1.700D 17	1.514D 06	9.071D 09	1.898D 12
4.00	7.973D-05	2.105D 08	2.711D 08	1.401D 10	1.029D 11	1.700D 17	1.049D 06	8.930D 09	1.898D 12
4.20	7.610D-05	2.119D 08	2.572D 08	1.402D 10	9.750D 10	1.700D 17	7.310D 05	8.788D 09	1.898D 12
4.40	7.260D-05	2.130D 08	2.441D 08	1.403D 10	9.256D 10	1.700D 17	5.131D 05	8.646D 09	1.898D 12
4.60	6.924D-05	2.141D 08	2.316D 08	1.405D 10	8.804D 10	1.700D 17	3.640D 05	8.506D 09	1.898D 12
4.80	6.601D-05	2.152D 08	2.197D 08	1.406D 10	8.388D 10	1.700D 17	2.618D 05	8.368D 09	1.898D 12
5.00	6.291D-05	2.161D 08	2.085D 08	1.407D 10	8.005D 10	1.700D 17	1.917D 05	8.231D 09	1.898D 12
5.20	5.993D-05	2.170D 08	1.978D 08	1.408D 10	7.651D 10	1.700D 17	1.437D 05	8.097D 09	1.898D 12
5.40	5.707D-05	2.178D 08	1.876D 08	1.409D 10	7.323D 10	1.700D 17	1.106D 05	7.966D 09	1.898D 12
5.60	5.432D-05	2.185D 08	1.780D 08	1.410D 10	7.018D 10	1.700D 17	8.783D 04	7.837D 09	1.898D 12
5.80	5.170D-05	2.192D 08	1.689D 08	1.410D 10	6.735D 10	1.700D 17	7.209D 04	7.712D 09	1.898D 12
6.00	4.918D-05	2.198D 08	1.602D 08	1.411D 10	6.470D 10	1.700D 17	6.116D 04	7.589D 09	1.898D 12
6.20	4.677D-05	2.204D 08	1.520D 08	1.412D 10	6.223D 10	1.700D 17	5.352D 04	7.469D 09	1.899D 12
6.40	4.447D-05	2.209D 08	1.442D 08	1.413D 10	5.992D 10	1.700D 17	4.814D 04	7.353D 09	1.899D 12
6.60	4.228D-05	2.213D 08	1.368D 08	1.413D 10	5.775D 10	1.700D 17	4.430D 04	7.239D 09	1.899D 12
6.80	4.018D-05	2.218D 08	1.298D 08	1.414D 10	5.571D 10	1.700D 17	4.151D 04	7.129D 09	1.899D 12
7.00	3.818D-05	2.221D 08	1.231D 08	1.415D 10	5.379D 10	1.700D 17	3.946D 04	7.021D 09	1.899D 12
7.20	3.628D-05	2.224D 08	1.168D 08	1.415D 10	5.199D 10	1.700D 17	3.789D 04	6.916D 09	1.899D 12
7.40	3.446D-05	2.227D 08	1.108D 08	1.416D 10	5.028D 10	1.700D 17	3.668D 04	6.815D 09	1.899D 12
7.60	3.273D-05	2.230D 08	1.051D 08	1.416D 10	4.867D 10	1.700D 17	3.569D 04	6.716D 09	1.899D 12
7.80	3.108D-05	2.232D 08	9.971D 07	1.417D 10	4.714D 10	1.700D 17	3.488D 04	6.619D 09	1.899D 12
8.00	2.951D-05	2.234D 08	9.459D 07	1.417D 10	4.570D 10	1.700D 17	3.418D 04	6.525D 09	1.899D 12
8.20	2.802D-05	2.236D 08	8.974D 07	1.418D 10	4.433D 10	1.700D 17	3.356D 04	6.434D 09	1.899D 12
8.40	2.660D-05	2.237D 08	8.514D 07	1.418D 10	4.303D 10	1.700D 17	3.300D 04	6.346D 09	1.899D 12
8.60	2.525D-05	2.239D 08	8.078D 07	1.419D 10	4.179D 10	1.700D 17	3.248D 04	6.259D 09	1.899D 12
8.80	2.397D-05	2.240D 08	7.664D 07	1.419D 10	4.061D 10	1.700D 17	3.200D 04	6.175D 09	1.899D 12
9.00	2.276D-05	2.241D 08	7.272D 07	1.420D 10	3.949D 10	1.700D 17	3.154D 04	6.093D 09	1.899D 12
9.20	2.160D-05	2.242D 08	6.900D 07	1.420D 10	3.842D 10	1.700D 17	3.110D 04	6.014D 09	1.900D 12
9.40	2.050D-05	2.242D 08	6.547D 07	1.420D 10	3.740D 10	1.700D 17	3.068D 04	5.936D 09	1.900D 12
9.60	1.946D-05	2.243D 08	6.213D 07	1.421D 10	3.642D 10	1.700D 17	3.027D 04	5.861D 09	1.900D 12
9.80	1.847D-05	2.244D 08	5.895D 07	1.421D 10	3.549D 10	1.700D 17	2.987D 04	5.788D 09	1.900D 12
10.00	1.753D-05	2.244D 08	5.595D 07	1.421D 10	3.459D 10	1.700D 17	2.949D 04	5.716D 09	1.900D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.3000D 07	1.4000D 09	1.0000D 06	8.0000D 05	3.5000D 09	4.0000D 08
0.20	2.3150D 12	2.2770D 08	1.7380D 06	8.5540D 08	1.7960D 09	1.0010D 06	9.8470D 05	3.3400D-04	8.4530D-05
0.40	1.8410D 12	2.4330D 08	3.1150D 06	1.1550D 09	1.7880D 09	1.0020D 06	1.3860D 06	3.4380D-04	6.4460D-05
0.60	1.5150D 12	2.3760D 08	4.8420D 06	1.3720D 09	1.7800D 09	1.0040D 06	1.8940D 06	3.9920D-04	6.2980D-05
0.80	1.2800D 12	2.2350D 08	6.7180D 06	1.5290D 09	1.7710D 09	1.0050D 06	2.4680D 06	4.3390D-04	6.1450D-05
1.00	1.1030D 12	2.0660D 08	8.6140D 06	1.6400D 09	1.7630D 09	1.0060D 06	3.0800D 06	4.5460D-04	6.0010D-05
1.20	9.6540D 11	1.8930D 08	1.0450D 07	1.7170D 09	1.7540D 09	1.0080D 06	3.7060D 06	4.6640D-04	5.8830D-05
1.40	8.5520D 11	1.7270D 08	1.2180D 07	1.7670D 09	1.7460D 09	1.0090D 06	4.3300D 06	4.7290D-04	5.7920D-05
1.60	7.6520D 11	1.5740D 08	1.3790D 07	1.7980D 09	1.7380D 09	1.0100D 06	4.9400D 06	4.7610D-04	5.7310D-05
1.80	6.9050D 11	1.4340D 08	1.5270D 07	1.8150D 09	1.7290D 09	1.0110D 06	5.5270D 06	4.7720D-04	5.6940D-05
2.00	6.2760D 11	1.3080D 08	1.6610D 07	1.8190D 09	1.7210D 09	1.0120D 06	6.0850D 06	4.7720D-04	5.6780D-05
2.20	5.7410D 11	1.1950D 08	1.7830D 07	1.8150D 09	1.7130D 09	1.0130D 06	6.6110D 06	4.7620D-04	5.6790D-05
2.40	5.2790D 11	1.0930D 08	1.8940D 07	1.8050D 09	1.7050D 09	1.0130D 06	7.1030D 06	4.7460D-04	5.6930D-05
2.60	4.8780D 11	1.0030D 08	1.9930D 07	1.7900D 09	1.6970D 09	1.0140D 06	7.5600D 06	4.7250D-04	5.7160D-05
2.80	4.5270D 11	9.2130D 07	2.0830D 07	1.7710D 09	1.6890D 09	1.0150D 06	7.9810D 06	4.6990D-04	5.7460D-05
3.00	4.2170D 11	8.4850D 07	2.1650D 07	1.7490D 09	1.6810D 09	1.0150D 06	8.3670D 06	4.6690D-04	5.7800D-05
3.20	3.9420D 11	7.8310D 07	2.2380D 07	1.7250D 09	1.6740D 09	1.0160D 06	8.7200D 06	4.6360D-04	5.8170D-05
3.40	3.6960D 11	7.2430D 07	2.3040D 07	1.7000D 09	1.6660D 09	1.0160D 06	9.0390D 06	4.5980D-04	5.8550D-05
3.60	3.4760D 11	6.7130D 07	2.3630D 07	1.6740D 09	1.6580D 09	1.0170D 06	9.3270D 06	4.5570D-04	5.8940D-05
3.80	3.2770D 11	6.2340D 07	2.4170D 07	1.6470D 09	1.6500D 09	1.0170D 06	9.5850D 06	4.5130D-04	5.9310D-05
4.00	3.0970D 11	5.8010D 07	2.4660D 07	1.6200D 09	1.6430D 09	1.0170D 06	9.8140D 06	4.4670D-04	5.9680D-05
4.20	2.9340D 11	5.4080D 07	2.5100D 07	1.5930D 09	1.6350D 09	1.0180D 06	1.0020D 07	4.4180D-04	6.0030D-05
4.40	2.7840D 11	5.0500D 07	2.5500D 07	1.5670D 09	1.6280D 09	1.0180D 06	1.0190D 07	4.3680D-04	6.0360D-05
4.60	2.6470D 11	4.7250D 07	2.5870D 07	1.5400D 09	1.6200D 09	1.0180D 06	1.0350D 07	4.3160D-04	6.0670D-05
4.80	2.5220D 11	4.4280D 07	2.6200D 07	1.5140D 09	1.6130D 09	1.0190D 06	1.0480D 07	4.2620D-04	6.0960D-05
5.00	2.4060D 11	4.1560D 07	2.6500D 07	1.4880D 09	1.6060D 09	1.0190D 06	1.0590D 07	4.2080D-04	6.1230D-05
5.20	2.2990D 11	3.9080D 07	2.6770D 07	1.4630D 09	1.5980D 09	1.0190D 06	1.0680D 07	4.1530D-04	6.1480D-05
5.40	2.2000D 11	3.6790D 07	2.7020D 07	1.4380D 09	1.5910D 09	1.0190D 06	1.0760D 07	4.0980D-04	6.1710D-05
5.60	2.1080D 11	3.4690D 07	2.7240D 07	1.4130D 09	1.5840D 09	1.0200D 06	1.0820D 07	4.0420D-04	6.1920D-05
5.80	2.0230D 11	3.2750D 07	2.7450D 07	1.3900D 09	1.5770D 09	1.0200D 06	1.0860D 07	3.9870D-04	6.2110D-05
6.00	1.9430D 11	3.0960D 07	2.7640D 07	1.3660D 09	1.5700D 09	1.0200D 06	1.0890D 07	3.9310D-04	6.2280D-05
6.20	1.8690D 11	2.9310D 07	2.7810D 07	1.3440D 09	1.5630D 09	1.0200D 06	1.0910D 07	3.8760D-04	6.2440D-05
6.40	1.7990D 11	2.7780D 07	2.7960D 07	1.3220D 09	1.5560D 09	1.0200D 06	1.0910D 07	3.8210D-04	6.2580D-05
6.60	1.7340D 11	2.6360D 07	2.8100D 07	1.3000D 09	1.5490D 09	1.0200D 06	1.0900D 07	3.7670D-04	6.2710D-05
6.80	1.6730D 11	2.5040D 07	2.8230D 07	1.2800D 09	1.5430D 09	1.0210D 06	1.0890D 07	3.7140D-04	6.2830D-05
7.00	1.6150D 11	2.3810D 07	2.8350D 07	1.2590D 09	1.5360D 09	1.0210D 06	1.0860D 07	3.6610D-04	6.2930D-05
7.20	1.5600D 11	2.2670D 07	2.8460D 07	1.2400D 09	1.5290D 09	1.0210D 06	1.0830D 07	3.6090D-04	6.3020D-05
7.40	1.5090D 11	2.1600D 07	2.8560D 07	1.2200D 09	1.5230D 09	1.0210D 06	1.0790D 07	3.5570D-04	6.3110D-05
7.60	1.4610D 11	2.0600D 07	2.8650D 07	1.2020D 09	1.5160D 09	1.0210D 06	1.0750D 07	3.5070D-04	6.3180D-05
7.80	1.4150D 11	1.9670D 07	2.8730D 07	1.1840D 09	1.5100D 09	1.0210D 06	1.0690D 07	3.4570D-04	6.3240D-05
8.00	1.3710D 11	1.8800D 07	2.8800D 07	1.1660D 09	1.5030D 09	1.0210D 06	1.0630D 07	3.4090D-04	6.3300D-05
8.20	1.3300D 11	1.7980D 07	2.8870D 07	1.1490D 09	1.4970D 09	1.0210D 06	1.0570D 07	3.3610D-04	6.3350D-05
8.40	1.2910D 11	1.7210D 07	2.8930D 07	1.1320D 09	1.4910D 09	1.0220D 06	1.0500D 07	3.3150D-04	6.3390D-05
8.60	1.2540D 11	1.6490D 07	2.8990D 07	1.1160D 09	1.4850D 09	1.0220D 06	1.0430D 07	3.2690D-04	6.3430D-05
8.80	1.2180D 11	1.5810D 07	2.9040D 07	1.1000D 09	1.4780D 09	1.0220D 06	1.0360D 07	3.2240D-04	6.3460D-05
9.00	1.1850D 11	1.5170D 07	2.9080D 07	1.0850D 09	1.4720D 09	1.0220D 06	1.0280D 07	3.1810D-04	6.3490D-05
9.20	1.1530D 11	1.4560D 07	2.9130D 07	1.0700D 09	1.4660D 09	1.0220D 06	1.0200D 07	3.1380D-04	6.3510D-05
9.40	1.1220D 11	1.3990D 07	2.9160D 07	1.0550D 09	1.4600D 09	1.0220D 06	1.0120D 07	3.0960D-04	6.3540D-05
9.60	1.0930D 11	1.3450D 07	2.9200D 07	1.0410D 09	1.4540D 09	1.0220D 06	1.0040D 07	3.0550D-04	6.3550D-05
9.80	1.0650D 11	1.2950D 07	2.9220D 07	1.0270D 09	1.4480D 09	1.0220D 06	9.9520D 06	3.0150D-04	6.3570D-05
10.00	1.0380D 11	1.2460D 07	2.9250D 07	1.0130D 09	1.4420D 09	1.0220D 06	9.8650D 06	2.9770D-04	6.3580D-05

T=250 K, H=30 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.94D-06	6.06D-14
2	2*NO3 >>> 2*NO2 + O2	4.71D-17	7.46D-62
3	NO2 + NO3 >>> NO2 + NO + O2	4.21D-15	1.19D-34
4	NO3 + NO >>> 2*NO2	1.90D-11	3.29D-32
5	NO + O3 >>> NO2 + O2	6.36D-15	1.08D-56
6	NO2 + O3 >>> NO3 + O2	6.65D-18	8.33D-39
7	HNO3 + M >>> HO + NO2 + M	2.57D-28	1.18D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.80D-29
9	O + O + M >>> O2 + M	1.29D-15	3.30D-58
10	O + O2 + M >>> O3 + M	2.76D-16	7.74D-17
11	O + O3 >>> 2*O2	1.92D-15	0.0
12	O + NO + M >>> NO2 + M	5.43D-14	4.02D-48
13	O + NO2 >>> NO + O2	5.12D-12	6.27D-53
14	O + NO2 + M >>> NO3 + M	3.39D-14	2.71D-24
15	HO + HO >>> H2O + O	1.09D-12	9.77D-27
16	O2 + 2*NO >>> 2*NO2	2.75D-38	3.88D-35
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	7.73D-25
19	O + HO2 >>> HO + O2	1.08D-11	5.45D-60
20	O2 + H + M >>> HO2 + M	1.33D-14	1.71D-31
21	O3 + H >>> HO + O2	1.27D-11	0.0
22	O3 + HO >>> HO2 + O2	2.75D-14	1.04D-48
23	O3 + HO2 >>> HO + 2*O2	4.45D-16	2.41D-68
24	H + HO + M >>> H2O + M	2.71D-13	0.0
25	H + HO2 >>> 2*HO	9.40D-12	1.62D-46
26	H + HO2 >>> H2 + O2	1.04D-11	2.55D-61
27	H + H2O >>> H2 + HO	2.34D-28	1.14D-15
28	H + H2O2 >>> H2 + HO2	8.36D-15	5.62D-29
29	H + H2O2 >>> HO + H2O	1.09D-14	1.35D-75
30	2*HO + M >>> H2O2 + M	1.55D-13	4.16D-32
31	HO + HO2 >>> H2O + O2	1.12D-11	3.89D-74
32	2*HO2 >>> H2O2 + O2	2.30D-12	8.58D-49
33	HO2 + H2O >>> H2O2 + HO	1.02D-39	5.49D-13
34	NO + H + M >>> HNO + M	8.43D-15	1.32D-33
35	NO + HO >>> NO2 + H	3.05D-38	3.01D-11
36	NO + HO + M >>> HNO2 + M	1.11D-12	4.20D-29
37	NO + HO2 >>> NO2 + HO	1.65D-13	7.47D-21
38	H + H + M >>> H2 + M	3.39D-16	0.0
39	HNO4 + M >>> HO2 + NO2 + M	5.80D-06	1.07D-13
40	CLNO3 + M >>> CLO + NO2 + M	1.56D-07	8.15D-14

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.0000D 08	4.2000D 09	3.0000D 06	4.5000D 08	2.5000D 12	7.8000D 16	4.0000D 08	3.0000D 06	1.2000D 12
0.20	4.0000D 08	4.2010D 09	3.0090D 06	4.4860D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.9910D 06	1.2000D 12
0.40	4.0000D 08	4.2030D 09	3.0180D 06	4.4710D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.9520D 06	1.2000D 12
0.60	4.0000D 08	4.2040D 09	3.0270D 06	4.4570D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.9140D 06	1.2000D 12
0.80	4.0000D 08	4.2060D 09	3.0350D 06	4.4430D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.8770D 06	1.2000D 12
1.00	4.0000D 08	4.2070D 09	3.0440D 06	4.4290D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.8400D 06	1.2000D 12
1.20	4.0000D 08	4.2080D 09	3.0530D 06	4.4150D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.8040D 06	1.2000D 12
1.40	4.0000D 08	4.2100D 09	3.0620D 06	4.4010D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.7680D 06	1.2000D 12
1.60	4.0000D 08	4.2110D 09	3.0710D 06	4.3870D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.7330D 06	1.2000D 12
1.80	4.0000D 08	4.2130D 09	3.0800D 06	4.3730D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.6990D 06	1.2000D 12
2.00	4.0000D 08	4.2140D 09	3.0890D 06	4.3590D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.6650D 06	1.2000D 12
2.20	4.0000D 08	4.2150D 09	3.0980D 06	4.3450D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.6310D 06	1.2000D 12
2.40	4.0000D 08	4.2170D 09	3.1070D 06	4.3310D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.5980D 06	1.2000D 12
2.60	4.0000D 08	4.2180D 09	3.1160D 06	4.3170D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.5650D 06	1.2000D 12
2.80	4.0000D 08	4.2190D 09	3.1250D 06	4.3030D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.5330D 06	1.2000D 12
3.00	4.0000D 08	4.2210D 09	3.1330D 06	4.2900D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.5020D 06	1.2000D 12
3.20	4.0000D 08	4.2220D 09	3.1420D 06	4.2760D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.4710D 06	1.2000D 12
3.40	4.0000D 08	4.2240D 09	3.1510D 06	4.2620D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.4400D 06	1.2000D 12
3.60	4.0000D 08	4.2250D 09	3.1600D 06	4.2490D 08	2.5000D 12	7.8000D 16	4.0000D 08	2.4100D 06	1.2000D 12
3.80	4.0000D 08	4.2260D 09	3.1690D 06	4.2350D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.3800D 06	1.2000D 12
4.00	4.0000D 08	4.2280D 09	3.1780D 06	4.2220D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.3510D 06	1.2000D 12
4.20	4.0000D 08	4.2290D 09	3.1870D 06	4.2080D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.3220D 06	1.2000D 12
4.40	4.0000D 08	4.2300D 09	3.1960D 06	4.1950D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.2940D 06	1.2000D 12
4.60	4.0000D 08	4.2310D 09	3.2050D 06	4.1810D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.2660D 06	1.2000D 12
4.80	4.0000D 08	4.2330D 09	3.2140D 06	4.1680D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.2380D 06	1.2000D 12
5.00	4.0000D 08	4.2340D 09	3.2230D 06	4.1550D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.2110D 06	1.2000D 12
5.20	4.0000D 08	4.2350D 09	3.2320D 06	4.1420D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.1840D 06	1.2000D 12
5.40	4.0000D 08	4.2370D 09	3.2410D 06	4.1280D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.1580D 06	1.2000D 12
5.60	4.0000D 08	4.2380D 09	3.2500D 06	4.1150D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.1320D 06	1.2000D 12
5.80	4.0000D 08	4.2390D 09	3.2590D 06	4.1020D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.1070D 06	1.2000D 12
6.00	4.0000D 08	4.2410D 09	3.2680D 06	4.0890D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.0810D 06	1.2000D 12
6.20	4.0000D 08	4.2420D 09	3.2770D 06	4.0760D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.0570D 06	1.2000D 12
6.40	4.0000D 08	4.2430D 09	3.2860D 06	4.0630D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.0320D 06	1.2000D 12
6.60	4.0000D 08	4.2440D 09	3.2950D 06	4.0500D 08	2.5000D 12	7.8000D 16	4.0010D 08	2.0080D 06	1.2000D 12
6.80	4.0000D 08	4.2460D 09	3.3040D 06	4.0370D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.9850D 06	1.2000D 12
7.00	4.0000D 08	4.2470D 09	3.3130D 06	4.0240D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.9610D 06	1.2000D 12
7.20	4.0000D 08	4.2480D 09	3.3220D 06	4.0110D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.9380D 06	1.2000D 12
7.40	4.0000D 08	4.2500D 09	3.3310D 06	3.9990D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.9160D 06	1.2000D 12
7.60	4.0000D 08	4.2510D 09	3.3410D 06	3.9860D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.8940D 06	1.2000D 12
7.80	4.0000D 08	4.2520D 09	3.3500D 06	3.9730D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.8720D 06	1.2000D 12
8.00	4.0000D 08	4.2530D 09	3.3590D 06	3.9610D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.8500D 06	1.2000D 12
8.20	4.0000D 08	4.2550D 09	3.3680D 06	3.9480D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.8290D 06	1.2000D 12
8.40	4.0000D 08	4.2560D 09	3.3770D 06	3.9350D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.8080D 06	1.2000D 12
8.60	4.0000D 08	4.2570D 09	3.3860D 06	3.9230D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.7870D 06	1.2000D 12
8.80	4.0000D 08	4.2590D 09	3.3950D 06	3.9100D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.7670D 06	1.2000D 12
9.00	4.0000D 08	4.2600D 09	3.4040D 06	3.8980D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.7470D 06	1.2000D 12
9.20	4.0000D 08	4.2610D 09	3.4130D 06	3.8850D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.7270D 06	1.2000D 12
9.40	4.0000D 08	4.2620D 09	3.4220D 06	3.8730D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.7080D 06	1.2000D 12
9.60	4.0000D 08	4.2630D 09	3.4320D 06	3.8610D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.6880D 06	1.2000D 12
9.80	4.0000D 08	4.2640D 09	3.4410D 06	3.8480D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.6700D 06	1.2000D 12
10.00	4.0000D 08	4.2660D 09	3.4500D 06	3.8360D 08	2.5000D 12	7.8000D 16	4.0010D 08	1.6510D 06	1.2000D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.5000D 07	1.2000D 09	1.0000D 06	8.0000D 05	1.5000D 09	2.0000D 08
0.20	1.3410D 04	1.6050D-03	1.0000D 06	2.6000D 07	1.2000D 09	1.0000D 06	8.0030D 05	1.5000D 09	2.0000D 08
0.40	1.4030D 02	2.4420D-05	1.0000D 06	2.6040D 07	1.2000D 09	1.0000D 06	8.0060D 05	1.5000D 09	2.0000D 08
0.60	2.9300D 00	3.4400D-06	1.0000D 06	2.6070D 07	1.2000D 09	1.0000D 06	8.0090D 05	1.5000D 09	2.0000D 08
0.80	5.4150D-01	3.1210D-06	1.0000D 06	2.6100D 07	1.2000D 09	1.0000D 06	8.0120D 05	1.5000D 09	2.0000D 08
1.00	4.9900D-01	3.0770D-06	1.0000D 06	2.6140D 07	1.2000D 09	1.0000D 06	8.0150D 05	1.5000D 09	2.0000D 08
1.20	4.8820D-01	3.0360D-06	1.0000D 06	2.6170D 07	1.2000D 09	1.0000D 06	8.0170D 05	1.5000D 09	2.0000D 08
1.40	4.7810D-01	2.9970D-06	1.0000D 06	2.6200D 07	1.2000D 09	1.0000D 06	8.0200D 05	1.5000D 09	2.0000D 08
1.60	4.6830D-01	2.9580D-06	1.0000D 06	2.6230D 07	1.2000D 09	1.0000D 06	8.0230D 05	1.5000D 09	2.0000D 08
1.80	4.5880D-01	2.9190D-06	1.0000D 06	2.6260D 07	1.2000D 09	1.0000D 06	8.0250D 05	1.5000D 09	2.0000D 08
2.00	4.4950D-01	2.8910D-06	1.0000D 06	2.6290D 07	1.2000D 09	1.0000D 06	8.0280D 05	1.5000D 09	2.0000D 08
2.20	4.4050D-01	2.8440D-06	1.0000D 06	2.6320D 07	1.2000D 09	1.0000D 06	6.0300D 05	1.5000D 09	2.0000D 08
2.40	4.3170D-01	2.8080D-06	1.0000D 06	2.6350D 07	1.2000D 09	1.0000D 06	8.0330D 05	1.5000D 09	2.0000D 08
2.60	4.2320D-01	2.7710D-06	1.0000D 06	2.6370D 07	1.2000D 09	1.0000D 06	8.0350D 05	1.5000D 09	2.0000D 08
2.80	4.1490D-01	2.7360D-06	1.0000D 06	2.6400D 07	1.2000D 09	1.0000D 06	8.0380D 05	1.5000D 09	2.0000D 08
3.00	4.0690D-01	2.7010D-06	1.0000D 06	2.6430D 07	1.2000D 09	1.0000D 06	8.0400D 05	1.5000D 09	2.0000D 08
3.20	3.9900D-01	2.6670D-06	1.0000D 06	2.6460D 07	1.2000D 09	1.0000D 06	8.0430D 05	1.5000D 09	2.0000D 08
3.40	3.9140D-01	2.6330D-06	1.0000D 06	2.6480D 07	1.2000D 09	1.0000D 06	8.0450D 05	1.5000D 09	2.0010D 08
3.60	3.8400D-01	2.6000D-06	1.0000D 06	2.6510D 07	1.2000D 09	1.0000D 06	8.0470D 05	1.5000D 09	2.0010D 08
3.80	3.7480D-01	2.5670D-06	1.0000D 06	2.6530D 07	1.2000D 09	1.0000D 06	8.0500D 05	1.5000D 09	2.0010D 08
4.00	3.6980D-01	2.5350D-06	1.0000D 06	2.6560D 07	1.2000D 09	1.0000D 06	8.0520D 05	1.5000D 09	2.0010D 08
4.20	3.6290D-01	2.5030D-06	1.0000D 06	2.6580D 07	1.2000D 09	1.0000D 06	8.0540D 05	1.5000D 09	2.0010D 08
4.40	3.5630D-01	2.4720D-06	1.0000D 06	2.6610D 07	1.2000D 09	1.0000D 06	8.0560D 05	1.5000D 09	2.0010D 08
4.60	3.4980D-01	2.4410D-06	1.0000D 06	2.6630D 07	1.2000D 09	1.0000D 06	8.0580D 05	1.5000D 09	2.0010D 08
4.80	3.4350D-01	2.4110D-06	1.0000D 06	2.6660D 07	1.2000D 09	1.0000D 06	8.0600D 05	1.5000D 09	2.0010D 08
5.00	3.3740D-01	2.3810D-06	1.0000D 06	2.6680D 07	1.2000D 09	1.0000D 06	8.0620D 05	1.5000D 09	2.0010D 08
5.20	3.3150D-01	2.3520D-06	1.0000D 06	2.6700D 07	1.2000D 09	1.0000D 06	8.0640D 05	1.5000D 09	2.0010D 08
5.40	3.2570D-01	2.3230D-06	1.0000D 06	2.6720D 07	1.2000D 09	1.0000D 06	8.0660D 05	1.5000D 09	2.0010D 08
5.60	3.2000D-01	2.2950D-06	1.0000D 06	2.6750D 07	1.2000D 09	1.0000D 06	8.0680D 05	1.5000D 09	2.0010D 08
5.80	3.1450D-01	2.2670D-06	1.0000D 06	2.6770D 07	1.2000D 09	1.0000D 06	8.0700D 05	1.5000D 09	2.0010D 08
6.00	3.0920D-01	2.2390D-06	1.0000D 05	2.6790D 07	1.2000D 09	1.0000D 06	8.0720D 05	1.5000D 09	2.0010D 08
6.20	3.0400D-01	2.2120D-06	1.0000D 06	2.6810D 07	1.2000D 09	1.0000D 06	8.0740D 05	1.5000D 09	2.0010D 08
6.40	2.9890D-01	2.1860D-06	1.0000D 06	2.6830D 07	1.2000D 09	1.0000D 06	8.0760D 05	1.5000D 09	2.0010D 08
6.60	2.9400D-01	2.1590D-06	1.0000D 06	2.6850D 07	1.2000D 09	1.0000D 06	8.0780D 05	1.5000D 09	2.0010D 08
6.80	2.8920D-01	2.1340D-06	1.0000D 06	2.6870D 07	1.2000D 09	1.0000D 06	8.0790D 05	1.5000D 09	2.0010D 08
7.00	2.8460D-01	2.1080D-06	1.0000D 06	2.6890D 07	1.2000D 09	1.0000D 06	8.0810D 05	1.5000D 09	2.0010D 08
7.20	2.8000D-01	2.0830D-06	1.0000D 06	2.6910D 07	1.2000D 09	1.0000D 06	8.0830D 05	1.5000D 09	2.0010D 08
7.40	2.7560D-01	2.0590D-06	1.0000D 06	2.6930D 07	1.2000D 09	1.0000D 06	8.0850D 05	1.5000D 09	2.0010D 08
7.60	2.7130D-01	2.0340D-06	1.0000D 06	2.6950D 07	1.2000D 09	1.0000D 06	8.0860D 05	1.5000D 09	2.0010D 08
7.80	2.6710D-01	2.0100D-06	1.0000D 06	2.6960D 07	1.2000D 09	1.0000D 06	8.0880D 05	1.5000D 09	2.0010D 08
8.00	2.6310D-01	1.9870D-06	1.0000D 06	2.6980D 07	1.2000D 09	1.0000D 06	8.0900D 05	1.5000D 09	2.0010D 08
8.20	2.5910D-01	1.9640D-06	1.0000D 06	2.7000D 07	1.2000D 09	1.0000D 06	8.0910D 05	1.5000D 09	2.0010D 08
8.40	2.5520D-01	1.9410D-06	1.0000D 06	2.7020D 07	1.2000D 09	1.0000D 06	8.0930D 05	1.5000D 09	2.0010D 08
8.60	2.5150D-01	1.9190D-06	1.0000D 06	2.7030D 07	1.2000D 09	1.0000D 06	8.0940D 05	1.5000D 09	2.0010D 08
8.80	2.4780D-01	1.8960D-06	1.0000D 06	2.7050D 07	1.2000D 09	1.0000D 06	8.0960D 05	1.5000D 09	2.0010D 08
9.00	2.4420D-01	1.8750D-06	1.0000D 06	2.7070D 07	1.2000D 09	1.0000D 06	8.0970D 05	1.5000D 09	2.0010D 08
9.20	2.4080D-01	1.8530D-06	1.0000D 06	2.7080D 07	1.2000D 09	1.0000D 06	8.0990D 05	1.5000D 09	2.0010D 08
9.40	2.3740D-01	1.8320D-06	1.0000D 06	2.7100D 07	1.2000D 09	1.0000D 06	8.1000D 05	1.5000D 09	2.0010D 08
9.60	2.3410D-01	1.8110D-06	1.0000D 06	2.7120D 07	1.2000D 09	1.0000D 06	8.1020D 05	1.5000D 09	2.0010D 08
9.80	2.3090D-01	1.7910D-06	1.0000D 06	2.7130D 07	1.2000D 09	1.0000D 06	8.1030D 05	1.5000D 09	2.0020D 08
10.00	2.2780D-01	1.7710D-06	1.0000D 06	2.7150D 07	1.2000D 09	1.0000D 06	8.1050D 05	1.5000D 09	2.0020D 08

T=300 K, H=30 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.570-03	2.840-14
2	2*NO3 >>> 2*NO2 + O2	2.410-16	1.750-58
3	NO2 + NO3 >>> NO2 + NO + O2	8.210-15	4.920-35
4	NO3 + NO >>> 2*NO2	1.900-11	6.980-29
5	NO + O3 >>> NO2 + O2	1.670-14	2.850-49
6	NO2 + O3 >>> NO3 + O2	3.410-17	2.000-34
7	HNO3 + M >>> HO + NO2 + M	1.920-21	6.220-13
8	HNO3 + HO >>> H2O + NO3	8.000-14	1.250-26
9	O + O + M >>> O2 + M	5.900-16	1.260-58
10	O + O2 + M >>> O3 + M	1.640-16	1.310-09
11	O + O3 >>> 2*O2	8.900-15	0.0
12	O + NO + M >>> NO2 + M	3.060-14	1.200-38
13	O + NO2 >>> NO + O2	6.250-12	3.730-46
14	O + NO2 + M >>> NO3 + M	2.820-14	2.260-24
15	HO + HO >>> H2O + O	1.570-12	4.630-24
16	O2 + 2*NO >>> 2*NO2	1.930-38	2.260-31
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.200-11	2.160-22
19	O + HO2 >>> HO + O2	1.510-11	8.510-52
20	O2 + H + M >>> HO2 + M	7.960-15	6.500-25
21	O3 + H >>> HO + O2	1.790-11	1.620-69
22	O3 + HO >>> HO2 + O2	5.350-14	8.980-43
23	O3 + HO2 >>> HO + 2*O2	1.040-15	1.530-63
24	H + HO + M >>> H2O + M	1.410-13	1.140-75
25	H + HO2 >>> 2*HO	1.770-11	1.140-40
26	H + HO2 >>> H2 + O2	1.310-11	6.800-53
27	H + H2O >>> H2 + HO	2.180-25	6.410-15
28	H + H2O2 >>> H2 + HO2	2.130-14	2.960-26
29	H + H2O2 >>> HO + H2O	2.760-14	2.950-65
30	2*HO + M >>> H2O2 + M	7.080-14	5.170-25
31	HO + HO2 >>> H2O + O2	1.570-11	1.980-63
32	2*HO2 >>> H2O2 + O2	3.210-12	1.980-42
33	HO2 + H2O >>> H2O2 + HO	6.110-35	8.570-13
34	NO + H + M >>> HNO + M	5.750-15	1.470-26
35	NO + HO >>> NO2 + H	7.190-34	4.920-11
36	NO + HO + M >>> HNO2 + M	4.410-13	2.470-22
37	NO + HO2 >>> NO2 + HO	3.660-13	3.740-19
38	H + H + M >>> H2 + M	2.820-16	2.430-69
39	HNO4 + M >>> HO2 + NO2 + M	3.880-03	4.650-14
40	CLNO3 + M >>> CLO + NO2 + M	2.280-04	3.940-14

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.000D 08	4.200D 09	3.000D 06	4.500D 08	2.500D 12	7.800D 16	4.000D 08	3.000D 06	1.200D 12
0.20	3.999D 08	4.205D 09	3.192D 06	4.463D 08	2.500D 12	7.800D 16	4.000D 08	2.999D 06	1.200D 12
0.40	3.997D 08	4.210D 09	3.383D 06	4.425D 08	2.500D 12	7.800D 16	4.000D 08	2.932D 06	1.200D 12
0.60	3.996D 08	4.215D 09	3.574D 06	4.388D 08	2.500D 12	7.800D 16	4.000D 08	2.868D 06	1.200D 12
0.80	3.995D 08	4.220D 09	3.765D 06	4.352D 08	2.500D 12	7.800D 16	4.000D 08	2.806D 06	1.200D 12
1.00	3.994D 08	4.225D 09	3.956D 06	4.316D 08	2.500D 12	7.800D 16	4.000D 08	2.747D 06	1.200D 12
1.20	3.992D 08	4.229D 09	4.146D 06	4.280D 08	2.500D 12	7.800D 16	4.000D 08	2.690D 06	1.200D 12
1.40	3.991D 08	4.234D 09	4.337D 06	4.244D 08	2.500D 12	7.800D 16	4.000D 08	2.635D 06	1.200D 12
1.60	3.990D 08	4.239D 09	4.527D 06	4.208D 08	2.500D 12	7.800D 16	4.000D 08	2.582D 06	1.200D 12
1.80	3.989D 08	4.244D 09	4.717D 06	4.173D 08	2.500D 12	7.800D 16	4.000D 08	2.531D 06	1.200D 12
2.00	3.987D 08	4.248D 09	4.906D 06	4.138D 08	2.500D 12	7.800D 16	4.000D 08	2.483D 06	1.200D 12
2.20	3.986D 08	4.253D 09	5.095D 06	4.104D 08	2.500D 12	7.800D 16	4.000D 08	2.436D 06	1.200D 12
2.40	3.985D 08	4.258D 09	5.285D 06	4.070D 08	2.500D 12	7.800D 16	4.000D 08	2.391D 06	1.200D 12
2.60	3.984D 08	4.262D 09	5.474D 06	4.036D 08	2.500D 12	7.800D 16	4.000D 08	2.348D 06	1.200D 12
2.80	3.982D 08	4.267D 09	5.663D 06	4.002D 08	2.500D 12	7.800D 16	4.000D 08	2.307D 06	1.200D 12
3.00	3.981D 08	4.271D 09	5.852D 06	3.969D 08	2.500D 12	7.800D 16	4.000D 08	2.268D 06	1.200D 12
3.20	3.980D 08	4.276D 09	6.040D 06	3.935D 08	2.500D 12	7.800D 16	4.000D 08	2.230D 06	1.200D 12
3.40	3.979D 08	4.280D 09	6.229D 06	3.903D 08	2.500D 12	7.800D 16	4.000D 08	2.194D 06	1.200D 12
3.60	3.978D 08	4.285D 09	6.417D 06	3.870D 08	2.500D 12	7.800D 16	4.000D 08	2.159D 06	1.200D 12
3.80	3.976D 08	4.289D 09	6.605D 06	3.838D 08	2.500D 12	7.800D 16	4.000D 08	2.127D 06	1.200D 12
4.00	3.975D 08	4.294D 09	6.793D 06	3.806D 08	2.500D 12	7.800D 16	4.000D 08	2.095D 06	1.200D 12
4.20	3.974D 08	4.298D 09	6.980D 06	3.774D 08	2.500D 12	7.800D 16	4.000D 08	2.065D 06	1.200D 12
4.40	3.973D 08	4.303D 09	7.168D 06	3.742D 08	2.500D 12	7.800D 16	4.000D 08	2.037D 06	1.200D 12
4.60	3.971D 08	4.307D 09	7.355D 06	3.711D 08	2.500D 12	7.800D 16	4.000D 08	2.010D 06	1.200D 12
4.80	3.970D 08	4.311D 09	7.543D 06	3.680D 08	2.500D 12	7.800D 16	4.000D 08	1.984D 06	1.200D 12
5.00	3.969D 08	4.315D 09	7.730D 06	3.649D 08	2.500D 12	7.800D 16	4.000D 08	1.959D 06	1.200D 12
5.20	3.968D 08	4.320D 09	7.917D 06	3.619D 08	2.500D 12	7.800D 16	4.000D 08	1.936D 06	1.200D 12
5.40	3.966D 08	4.324D 09	8.103D 06	3.589D 08	2.500D 12	7.800D 16	4.000D 08	1.914D 06	1.200D 12
5.60	3.965D 08	4.328D 09	8.290D 06	3.559D 08	2.500D 12	7.800D 16	4.000D 08	1.894D 06	1.200D 12
5.80	3.964D 08	4.332D 09	8.477D 06	3.529D 08	2.500D 12	7.800D 16	4.000D 08	1.874D 06	1.200D 12
6.00	3.963D 08	4.337D 09	8.663D 06	3.499D 08	2.500D 12	7.800D 16	4.000D 08	1.856D 06	1.200D 12
6.20	3.961D 08	4.341D 09	8.849D 06	3.470D 08	2.500D 12	7.800D 16	4.000D 08	1.838D 06	1.200D 12
6.40	3.960D 08	4.345D 09	9.036D 06	3.441D 08	2.500D 12	7.800D 16	4.000D 08	1.822D 06	1.200D 12
6.60	3.959D 08	4.349D 09	9.222D 06	3.412D 08	2.500D 12	7.800D 16	4.000D 08	1.807D 06	1.200D 12
6.80	3.958D 08	4.353D 09	9.408D 06	3.384D 08	2.500D 12	7.800D 16	4.000D 08	1.792D 06	1.200D 12
7.00	3.956D 08	4.357D 09	9.593D 06	3.355D 08	2.500D 12	7.800D 16	4.000D 08	1.779D 06	1.200D 12
7.20	3.955D 08	4.361D 09	9.779D 06	3.327D 08	2.500D 12	7.800D 16	4.000D 08	1.767D 06	1.200D 12
7.40	3.954D 08	4.365D 09	9.965D 06	3.300D 08	2.500D 12	7.800D 16	4.000D 08	1.756D 06	1.200D 12
7.60	3.953D 08	4.369D 09	1.015D 07	3.272D 08	2.500D 12	7.800D 16	4.000D 08	1.745D 06	1.200D 12
7.80	3.951D 08	4.373D 09	1.034D 07	3.245D 08	2.500D 12	7.800D 16	4.000D 08	1.736D 06	1.200D 12
8.00	3.950D 08	4.377D 09	1.052D 07	3.217D 08	2.500D 12	7.800D 16	4.000D 08	1.727D 06	1.200D 12
8.20	3.949D 08	4.381D 09	1.071D 07	3.191D 08	2.500D 12	7.800D 16	4.000D 08	1.719D 06	1.200D 12
8.40	3.948D 08	4.384D 09	1.089D 07	3.164D 08	2.500D 12	7.800D 16	4.000D 08	1.712D 06	1.200D 12
8.60	3.947D 08	4.388D 09	1.108D 07	3.137D 08	2.500D 12	7.800D 16	4.000D 08	1.705D 06	1.200D 12
8.80	3.945D 08	4.392D 09	1.126D 07	3.111D 08	2.500D 12	7.800D 16	4.000D 08	1.700D 06	1.200D 12
9.00	3.944D 08	4.396D 09	1.145D 07	3.085D 08	2.500D 12	7.800D 16	4.001D 08	1.695D 06	1.200D 12
9.20	3.943D 08	4.400D 09	1.163D 07	3.059D 08	2.500D 12	7.800D 16	4.001D 08	1.691D 06	1.200D 12
9.40	3.942D 08	4.403D 09	1.182D 07	3.034D 08	2.500D 12	7.800D 16	4.001D 08	1.687D 06	1.200D 12
9.60	3.940D 08	4.407D 09	1.200D 07	3.008D 08	2.500D 12	7.800D 16	4.001D 08	1.685D 06	1.200D 12
9.80	3.939D 08	4.411D 09	1.218D 07	2.983D 08	2.500D 12	7.800D 16	4.001D 08	1.682D 06	1.200D 12
10.00	3.938D 08	4.415D 09	1.237D 07	2.958D 08	2.500D 12	7.800D 16	4.001D 08	1.681D 06	1.200D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.000D 06	1.000D 06	1.000D 06	2.500D 07	1.200D 09	1.000D 06	8.000D 05	1.500D 09	2.000D 08
0.20	7.721D 04	1.492D-02	1.000D 06	2.716D 07	1.200D 09	1.000D 06	8.001D 05	1.499D 09	2.000D 08
0.40	6.181D 03	1.193D-03	1.000D 06	2.839D 07	1.200D 09	1.000D 06	8.002D 05	1.498D 09	2.000D 08
0.60	7.133D 02	1.583D-04	1.000D 06	2.961D 07	1.200D 09	1.000D 06	8.003D 05	1.497D 09	2.000D 08
0.80	2.924D 02	7.890D-05	1.000D 06	3.082D 07	1.200D 09	1.000D 06	8.005D 05	1.495D 09	2.000D 08
1.00	2.600D 02	7.150D-05	1.000D 06	3.204D 07	1.200D 09	1.000D 06	8.006D 05	1.494D 09	2.000D 08
1.20	2.574D 02	6.957D-05	1.000D 06	3.325D 07	1.200D 09	1.000D 06	8.007D 05	1.493D 09	2.000D 08
1.40	2.572D 02	6.812D-05	1.000D 06	3.446D 07	1.200D 09	1.000D 06	8.008D 05	1.492D 09	1.999D 08
1.60	2.571D 02	6.674D-05	1.000D 06	3.566D 07	1.200D 09	1.000D 06	8.009D 05	1.491D 09	1.999D 08
1.80	2.571D 02	6.543D-05	1.000D 06	3.686D 07	1.200D 09	1.000D 06	8.010D 05	1.490D 09	1.999D 08
2.00	2.571D 02	6.416D-05	1.000D 06	3.806D 07	1.200D 09	1.000D 06	8.011D 05	1.488D 09	1.999D 08
2.20	2.571D 02	6.295D-05	1.000D 06	3.926D 07	1.200D 09	1.000D 06	8.011D 05	1.487D 09	1.999D 08
2.40	2.570D 02	6.179D-05	1.000D 06	4.045D 07	1.200D 09	1.000D 06	8.012D 05	1.486D 09	1.999D 08
2.60	2.570D 02	6.067D-05	1.000D 06	4.164D 07	1.200D 09	1.000D 06	8.013D 05	1.485D 09	1.999D 08
2.80	2.570D 02	5.961D-05	1.000D 06	4.282D 07	1.200D 09	1.000D 06	8.014D 05	1.484D 09	1.999D 08
3.00	2.569D 02	5.859D-05	1.000D 06	4.401D 07	1.200D 09	1.000D 06	8.015D 05	1.483D 09	1.999D 08
3.20	2.569D 02	5.761D-05	1.000D 06	4.519D 07	1.200D 09	1.000D 06	8.016D 05	1.482D 09	1.999D 08
3.40	2.569D 02	5.667D-05	1.000D 06	4.637D 07	1.200D 09	1.000D 06	8.016D 05	1.480D 09	1.999D 08
3.60	2.569D 02	5.578D-05	1.000D 06	4.754D 07	1.200D 09	1.000D 06	8.017D 05	1.479D 09	1.999D 08
3.80	2.569D 02	5.493D-05	1.000D 06	4.872D 07	1.200D 09	1.000D 06	8.018D 05	1.478D 09	1.999D 08
4.00	2.568D 02	5.411D-05	1.000D 06	4.989D 07	1.200D 09	1.000D 06	8.018D 05	1.477D 09	1.998D 08
4.20	2.568D 02	5.334D-05	1.000D 06	5.106D 07	1.200D 09	1.000D 06	8.019D 05	1.476D 09	1.998D 08
4.40	2.568D 02	5.260D-05	1.000D 06	5.222D 07	1.200D 09	1.000D 06	8.020D 05	1.475D 09	1.998D 08
4.60	2.568D 02	5.190D-05	1.000D 06	5.338D 07	1.200D 09	1.000D 06	8.021D 05	1.474D 09	1.998D 08
4.80	2.568D 02	5.123D-05	1.000D 06	5.454D 07	1.200D 09	1.000D 06	8.021D 05	1.472D 09	1.998D 08
5.00	2.568D 02	5.060D-05	1.000D 06	5.570D 07	1.200D 09	1.000D 06	8.022D 05	1.471D 09	1.998D 08
5.20	2.568D 02	5.000D-05	1.000D 06	5.686D 07	1.200D 09	1.000D 06	8.022D 05	1.470D 09	1.998D 08
5.40	2.567D 02	4.943D-05	1.000D 06	5.801D 07	1.200D 09	1.000D 06	8.023D 05	1.469D 09	1.998D 08
5.60	2.567D 02	4.889D-05	1.000D 06	5.916D 07	1.200D 09	1.000D 06	8.024D 05	1.468D 09	1.998D 08
5.80	2.567D 02	4.838D-05	1.000D 06	6.031D 07	1.200D 09	1.000D 06	8.024D 05	1.467D 09	1.998D 08
6.00	2.567D 02	4.791D-05	1.000D 06	6.146D 07	1.200D 09	1.000D 06	8.025D 05	1.466D 09	1.998D 08
6.20	2.567D 02	4.746D-05	1.000D 06	6.260D 07	1.200D 09	1.000D 06	8.025D 05	1.464D 09	1.998D 08
6.40	2.567D 02	4.704D-05	1.000D 06	6.374D 07	1.200D 09	1.000D 06	8.026D 05	1.463D 09	1.998D 08
6.60	2.567D 02	4.664D-05	1.000D 06	6.489D 07	1.200D 09	1.000D 06	8.026D 05	1.462D 09	1.997D 08
6.80	2.567D 02	4.627D-05	1.000D 06	6.602D 07	1.200D 09	1.000D 06	8.027D 05	1.461D 09	1.997D 08
7.00	2.567D 02	4.593D-05	1.000D 06	6.716D 07	1.200D 09	1.000D 06	8.028D 05	1.460D 09	1.997D 08
7.20	2.567D 02	4.561D-05	1.000D 06	6.829D 07	1.200D 09	1.000D 06	8.028D 05	1.459D 09	1.997D 08
7.40	2.567D 02	4.532D-05	1.000D 06	6.942D 07	1.200D 09	1.000D 06	8.029D 05	1.458D 09	1.997D 08
7.60	2.567D 02	4.505D-05	1.000D 06	7.055D 07	1.200D 09	1.000D 06	8.029D 05	1.457D 09	1.997D 08
7.80	2.567D 02	4.480D-05	1.000D 06	7.168D 07	1.200D 09	1.000D 06	8.030D 05	1.455D 09	1.997D 08
8.00	2.566D 02	4.457D-05	1.000D 06	7.281D 07	1.200D 09	1.000D 06	8.030D 05	1.454D 09	1.997D 08
8.20	2.566D 02	4.437D-05	1.000D 06	7.393D 07	1.200D 09	1.000D 06	8.031D 05	1.453D 09	1.997D 08
8.40	2.566D 02	4.418D-05	1.000D 06	7.505D 07	1.200D 09	1.000D 06	8.031D 05	1.452D 09	1.997D 08
8.60	2.566D 02	4.402D-05	1.000D 06	7.617D 07	1.200D 09	1.000D 06	8.032D 05	1.451D 09	1.997D 08
8.80	2.565D 02	4.387D-05	1.000D 06	7.729D 07	1.200D 09	1.000D 06	8.032D 05	1.450D 09	1.997D 08
9.00	2.566D 02	4.375D-05	1.000D 06	7.841D 07	1.200D 09	1.000D 06	8.032D 05	1.449D 09	1.997D 08
9.20	2.565D 02	4.364D-05	1.000D 06	7.952D 07	1.200D 09	1.000D 06	8.033D 05	1.448D 09	1.997D 08
9.40	2.566D 02	4.355D-05	1.000D 06	8.063D 07	1.200D 09	1.000D 06	8.033D 05	1.446D 09	1.996D 08
9.60	2.566D 02	4.348D-05	1.000D 06	8.175D 07	1.200D 09	1.000D 06	8.034D 05	1.445D 09	1.996D 08
9.80	2.566D 02	4.342D-05	1.000D 06	8.285D 07	1.200D 09	1.000D 06	8.034D 05	1.444D 09	1.996D 08
10.00	2.566D 02	4.338D-05	1.000D 06	8.396D 07	1.200D 09	1.000D 06	8.035D 05	1.443D 09	1.996D 08

T=700 K, H=30 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	2.30D 05	2.36D-15
2	2*NO3 >>> 2*NO2 + O2	2.57D-14	7.44D-49
3	NO2 + NO3 >>> NO2 + NO + O2	5.51D-14	3.97D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.23D-19
5	NO + O3 >>> NO2 + O2	2.65D-13	4.54D-28
6	NO2 + O3 >>> NO3 + O2	3.62D-15	6.56D-22
7	HNO3 + M >>> HO + NO2 + M	1.92D-02	3.21D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	4.74D-19
9	O + O + M >>> O2 + M	4.55D-17	1.42D-21
10	O + O2 + M >>> O3 + M	2.66D-17	1.61D 00
11	O + O3 >>> 2*O2	7.11D-13	8.63D-43
12	O + NO + M >>> NO2 + M	4.32D-15	1.02D-11
13	O + NO2 >>> NO + O2	1.11D-11	8.50D-27
14	O + NO2 + M >>> NO3 + M	1.21D-14	9.68D-25
15	HO + HO >>> H2O + O	4.53D-12	2.04D-16
16	O2 + 2*NO >>> 2*NO2	7.04D-39	9.37D-21
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.11D-15
19	O + HO2 >>> HO + O2	3.91D-11	2.19D-28
20	O2 + H + M >>> HO2 + M	1.32D-15	2.96D-06
21	O3 + H >>> HO + O2	4.78D-11	5.62D-37
22	O3 + HO >>> HO2 + O2	3.59D-13	8.31D-26
23	O3 + HO2 >>> HO + 2*O2	1.18D-14	1.12D-49
24	H + HO + M >>> H2O + M	6.67D-15	1.60D-27
25	H + HO2 >>> 2*HO	1.08D-10	5.87D-24
26	H + HO2 >>> H2 + O2	2.55D-11	8.03D-20
27	H + H2O >>> H2 + HO	6.56D-17	8.90D-13
28	H + H2O2 >>> H2 + HO2	3.06D-13	1.77D-18
29	H + H2O2 >>> HO + H2O	3.98D-13	1.02D-[illegible]3
30	2*HO + M >>> H2O2 + M	5.47D-15	5.00D-05
31	HO + HO2 >>> H2O + O2	4.06D-11	7.73D-33
32	2*HO2 >>> H2O2 + O2	8.32D-12	3.02D-24
33	HO2 + H2O >>> H2O2 + HO	2.72D-21	3.07D-12
34	NO + H + M >>> HNO + M	1.39D-15	1.05D-06
35	NO + HO >>> NO2 + H	2.23D-21	2.02D-10
36	NO + HO + M >>> HNO2 + M	2.28D-14	2.84D-03
37	NO + HO2 >>> NO2 + HO	3.60D-12	2.68D-14
38	H + H + M >>> H2 + M	1.21D-16	1.01D-25
39	HNO4 + M >>> HO2 + NO2 + M	3.35D 05	3.13D-15
40	CLNO3 + M >>> CLO + NO2 + M	1.80D 05	1.27D-15

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.0000D 09	4.2000D 09	3.0000D 06	4.5000D 08	2.5000D 12	7.8000D 16	4.0000D 08	3.0000D 06	1.2000D 12
0.20	1.4680D-02	3.4690D 09	4.1190D 08	3.2740D 09	1.8440D 12	7.8000D 16	3.9850D 08	1.0560D 09	1.2000D 12
0.40	5.0770D-03	1.2040D 09	4.1020D 08	5.5410D 09	1.4270D 12	7.8000D 16	3.9700D 08	1.1290D 09	1.2000D 12
0.60	2.1210D-03	5.1210D 08	4.0290D 08	6.2430D 09	1.1620D 12	7.8000D 16	3.9540D 08	1.1570D 09	1.2000D 12
0.80	1.3250D-03	3.2700D 08	3.9420D 08	6.4380D 09	9.8530D 11	7.8000D 16	3.9390D 08	1.1890D 09	1.2000D 12
1.00	1.0740D-03	2.7130D 08	3.8530D 08	6.5040D 09	8.6030D 11	7.8000D 16	3.9240D 08	1.2210D 09	1.2000D 12
1.20	9.7150D-04	2.5120D 08	3.7630D 08	6.5340D 09	7.6690D 11	7.8000D 16	3.9090D 08	1.2520D 09	1.2000D 12
1.40	9.1700D-04	2.4280D 08	3.6750D 08	6.5530D 09	6.9370D 11	7.8000D 16	3.8940D 08	1.2800D 09	1.2000D 12
1.60	8.8170D-04	2.3900D 08	3.5890D 08	6.5670D 09	6.3420D 11	7.8000D 16	3.8790D 08	1.3050D 09	1.2000D 12
1.80	8.5540D-04	2.3750D 08	3.5040D 08	6.5780D 09	5.8460D 11	7.8000D 16	3.8640D 08	1.3280D 09	1.2000D 12
2.00	8.3370D-04	2.3710D 08	3.4210D 08	6.5890D 09	5.4240D 11	7.8000D 16	3.8490D 08	1.3480D 09	1.2000D 12
2.20	8.1460D-04	2.3740D 08	3.3390D 08	6.5980D 09	5.0580D 11	7.8000D 16	3.8340D 08	1.3660D 09	1.2000D 12
2.40	7.9700D-04	2.3790D 08	3.2590D 08	6.6070D 09	4.7380D 11	7.8000D 16	3.8200D 08	1.3820D 09	1.2000D 12
2.60	7.8030D-04	2.3870D 08	3.1810D 08	6.6150D 09	4.4550D 11	7.8000D 16	3.8050D 08	1.3960D 09	1.2000D 12
2.80	7.6430D-04	2.3950D 08	3.1050D 08	6.6230D 09	4.2030D 11	7.8000D 16	3.7900D 08	1.4080D 09	1.2000D 12
3.00	7.4870D-04	2.4040D 08	3.0300D 08	6.6310D 09	3.9770D 11	7.8000D 16	3.7760D 08	1.4190D 09	1.2000D 12
3.20	7.3340D-04	2.4130D 08	2.9570D 08	6.6390D 09	3.7730D 11	7.8000D 16	3.7610D 08	1.4280D 09	1.2000D 12
3.40	7.1850D-04	2.4230D 08	2.8860D 08	6.6470D 09	3.5880D 11	7.8000D 16	3.7470D 08	1.4360D 09	1.2000D 12
3.60	7.0380D-04	2.4320D 08	2.8160D 08	6.6540D 09	3.4200D 11	7.8000D 16	3.7320D 08	1.4430D 09	1.2000D 12
3.80	6.8930D-04	2.4410D 08	2.7470D 08	6.6620D 09	3.2660D 11	7.8000D 16	3.7180D 08	1.4500D 09	1.2000D 12
4.00	6.7510D-04	2.4500D 08	2.6810D 08	6.6690D 09	3.1240D 11	7.8000D 16	3.7040D 08	1.4550D 09	1.2000D 12
4.20	6.6100D-04	2.4590D 08	2.6160D 08	6.6760D 09	2.9940D 11	7.8000D 16	3.6890D 08	1.4590D 09	1.2000D 12
4.40	6.4720D-04	2.4680D 08	2.5520D 08	6.6830D 09	2.8740D 11	7.8000D 16	3.6750D 08	1.4630D 09	1.2000D 12
4.60	6.3360D-04	2.4760D 08	2.4900D 08	6.6890D 09	2.7620D 11	7.8000D 16	3.6610D 08	1.4660D 09	1.2000D 12
4.80	6.2020D-04	2.4840D 08	2.4290D 08	6.6960D 09	2.6580D 11	7.8000D 16	3.6470D 08	1.4680D 09	1.2000D 12
5.00	6.0700D-04	2.4920D 08	2.3700D 08	6.7030D 09	2.5610D 11	7.8000D 16	3.6330D 08	1.4700D 09	1.2000D 12
5.20	5.9400D-04	2.5000D 08	2.3120D 08	6.7090D 09	2.4710D 11	7.8000D 16	3.6190D 08	1.4710D 09	1.2000D 12
5.40	5.8120D-04	2.5080D 08	2.2550D 08	6.7150D 09	2.3860D 11	7.8000D 16	3.6050D 08	1.4710D 09	1.2000D 12
5.60	5.6850D-04	2.5150D 08	2.2000D 08	6.7210D 09	2.3070D 11	7.8000D 16	3.5910D 08	1.4710D 09	1.2000D 12
5.80	5.5620D-04	2.5220D 08	2.1460D 08	6.7270D 09	2.2320D 11	7.8000D 16	3.5770D 08	1.4710D 09	1.2000D 12
6.00	5.4400D-04	2.5290D 08	2.0930D 08	6.7330D 09	2.1620D 11	7.8000D 16	3.5640D 08	1.4710D 09	1.2000D 12
6.20	5.3210D-04	2.5360D 08	2.0410D 08	6.7390D 09	2.0960D 11	7.8000D 16	3.5500D 08	1.4690D 09	1.2000D 12
6.40	5.2030D-04	2.5420D 08	1.9910D 08	6.7450D 09	2.0330D 11	7.8000D 16	3.5360D 08	1.4680D 09	1.2000D 12
6.60	5.0870D-04	2.5490D 08	1.9420D 08	6.7500D 09	1.9740D 11	7.8000D 16	3.5230D 08	1.4660D 09	1.2000D 12
6.80	4.9740D-04	2.5550D 08	1.8940D 08	6.7560D 09	1.9180D 11	7.8000D 16	3.5090D 08	1.4640D 09	1.2000D 12
7.00	4.8620D-04	2.5610D 08	1.8470D 08	6.7610D 09	1.8650D 11	7.8000D 16	3.4960D 08	1.4620D 09	1.2000D 12
7.20	4.7520D-04	2.5660D 08	1.8020D 08	6.7670D 09	1.8140D 11	7.8000D 16	3.4820D 08	1.4600D 09	1.2000D 12
7.40	4.6450D-04	2.5720D 08	1.7570D 08	6.7720D 09	1.7660D 11	7.8000D 16	3.4690D 08	1.4570D 09	1.2000D 12
7.60	4.5390D-04	2.5770D 08	1.7140D 08	6.7770D 09	1.7200D 11	7.8000D 16	3.4550D 08	1.4540D 09	1.2000D 12
7.80	4.4350D-04	2.5820D 08	1.6710D 08	6.7820D 09	1.6760D 11	7.8000D 16	3.4420D 08	1.4510D 09	1.2000D 12
8.00	4.3340D-04	2.5870D 08	1.6300D 08	6.7870D 09	1.6350D 11	7.8000D 16	3.4290D 08	1.4470D 09	1.2000D 12
8.20	4.2340D-04	2.5920D 08	1.5900D 08	6.7920D 09	1.5950D 11	7.8000D 16	3.4160D 08	1.4440D 09	1.2000D 12
8.40	4.1360D-04	2.5960D 08	1.5500D 08	6.7960D 09	1.5570D 11	7.8000D 16	3.4030D 08	1.4400D 09	1.2000D 12
8.60	4.0410D-04	2.6010D 08	1.5120D 08	6.8010D 09	1.5200D 11	7.8000D 16	3.3890D 08	1.4370D 09	1.2000D 12
8.80	3.9470D-04	2.6050D 08	1.4740D 08	6.8060D 09	1.4850D 11	7.8000D 16	3.3760D 08	1.4330D 09	1.2000D 12
9.00	3.8550D-04	2.6090D 08	1.4380D 08	6.8100D 09	1.4520D 11	7.8000D 16	3.3630D 08	1.4290D 09	1.2000D 12
9.20	3.7650D-04	2.6130D 08	1.4020D 08	6.8150D 09	1.4200D 11	7.8000D 16	3.3500D 08	1.4240D 09	1.2000D 12
9.40	3.6760D-04	2.6170D 08	1.3670D 08	6.8190D 09	1.3890D 11	7.8000D 16	3.3380D 08	1.4200D 09	1.2000D 12
9.60	3.5900D-04	2.6200D 08	1.3330D 08	6.8230D 09	1.3590D 11	7.8000D 16	3.3250D 08	1.4160D 09	1.2000D 12
9.80	3.5050D-04	2.6240D 08	1.3000D 08	6.8270D 09	1.3300D 11	7.8000D 16	3.3120D 08	1.4110D 09	1.2000D 12
10.00	3.4220D-04	2.6270D 08	1.2670D 08	6.8320D 09	1.3030D 11	7.8000D 16	3.2990D 08	1.4070D 09	1.2000D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	2.5000D 07	1.2000D 09	1.0000D 06	8.0000D 05	1.5000D 09	2.0000D 08
0.20	4.8270D 11	5.9430D 07	1.0800D 06	4.3640D 08	1.2010D 09	1.0000D 06	8.0520D 05	1.4150D-02	6.0110D-03
0.40	5.2830D 11	8.8470D 07	1.2400D 06	3.8840D 08	1.2010D 09	1.0000D 06	8.2810D 05	4.3730D-03	2.0870D-03
0.60	6.5000D 11	9.7670D 07	1.4390D 06	4.0800D 08	1.2000D 09	1.0000D 06	8.5860D 05	1.9530D-03	8.8740D-04
0.80	6.2520D 11	9.9240D 07	1.6580D 06	4.2830D 08	1.1990D 09	1.0000D 06	8.9210D 05	1.3090D-03	5.6670D-04
1.00	5.8510D 11	9.7290D 07	1.8860D 06	4.4730D 08	1.1990D 09	1.0010D 06	9.2720D 05	1.1350D-03	4.7020D-04
1.20	5.4220D 11	9.3800D 07	2.1160D 06	4.6460D 08	1.1980D 09	1.0010D 06	9.6350D 05	1.0910D-03	4.3530D-04
1.40	5.0150D 11	8.9740D 07	2.3450D 06	4.8010D 08	1.1980D 09	1.0010D 06	1.0010D 06	1.0890D-03	4.2070D-04
1.60	4.6450D 11	8.5590D 07	2.5690D 06	4.9390D 08	1.1970D 09	1.0010D 06	1.0390D 06	1.1040D-03	4.1430D-04
1.80	4.3160D 11	8.1550D 07	2.7890D 06	5.0630D 08	1.1960D 09	1.0010D 06	1.0780D 06	1.1240D-03	4.1160D-04
2.00	4.0250D 11	7.7730D 07	3.0030D 06	5.1730D 08	1.1960D 09	1.0010D 06	1.1170D 06	1.1470D-03	4.1100D-04
2.20	3.7670D 11	7.4150D 07	3.2110D 06	5.2710D 08	1.1950D 09	1.0020D 06	1.1570D 06	1.1700D-03	4.1130D-04
2.40	3.5380D 11	7.0810D 07	3.4130D 06	5.3590D 08	1.1950D 09	1.0020D 06	1.1980D 06	1.1920D-03	4.1230D-04
2.60	3.3330D 11	6.7700D 07	3.6090D 06	5.4360D 08	1.1940D 09	1.0020D 06	1.2390D 06	1.2130D-03	4.1360D-04
2.80	3.1500D 11	6.4810D 07	3.7980D 06	5.5060D 08	1.1940D 09	1.0020D 06	1.2810D 06	1.2330D-03	4.1510D-04
3.00	2.9840D 11	6.2110D 07	3.9820D 06	5.5680D 08	1.1930D 09	1.0020D 06	1.3230D 06	1.2510D-03	4.1660D-04
3.20	2.8350D 11	5.9590D 07	4.1600D 06	5.6220D 08	1.1930D 09	1.0020D 06	1.3650D 06	1.2680D-03	4.1820D-04
3.40	2.6980D 11	5.7230D 07	4.3320D 06	5.6710D 08	1.1920D 09	1.0020D 06	1.4080D 06	1.2840D-03	4.1980D-04
3.60	2.5740D 11	5.5020D 07	4.4980D 06	5.7140D 08	1.1920D 09	1.0020D 06	1.4500D 06	1.2990D-03	4.2140D-04
3.80	2.4600D 11	5.2940D 07	4.6600D 06	5.7520D 08	1.1910D 09	1.0020D 06	1.4940D 06	1.3120D-03	4.2300D-04
4.00	2.3550D 11	5.0990D 07	4.8160D 06	5.7850D 08	1.1900D 09	1.0030D 06	1.5370D 06	1.3250D-03	4.2460D-04
4.20	2.2590D 11	4.9150D 07	4.9670D 06	5.8140D 08	1.1900D 09	1.0030D 06	1.5800D 06	1.3360D-03	4.2610D-04
4.40	2.1690D 11	4.7410D 07	5.1130D 06	5.8390D 08	1.1890D 09	1.0030D 06	1.6240D 06	1.3470D-03	4.2760D-04
4.60	2.0860D 11	4.5770D 07	5.2550D 06	5.8600D 08	1.1890D 09	1.0030D 06	1.6680D 06	1.3560D-03	4.2910D-04
4.80	2.0090D 11	4.4220D 07	5.3920D 06	5.8780D 08	1.1880D 09	1.0030D 06	1.7110D 06	1.3650D-03	4.3050D-04
5.00	1.9370D 11	4.2750D 07	5.5250D 06	5.8930D 08	1.1880D 09	1.0030D 06	1.7550D 06	1.3730D-03	4.3190D-04
5.20	1.8690D 11	4.1360D 07	5.6530D 06	5.9050D 08	1.1870D 09	1.0030D 06	1.7990D 06	1.3800D-03	4.3330D-04
5.40	1.8060D 11	4.0030D 07	5.7780D 06	5.9150D 08	1.1870D 09	1.0030D 06	1.8430D 06	1.3870D-03	4.3460D-04
5.60	1.7460D 11	3.8770D 07	5.8990D 06	5.9220D 08	1.1860D 09	1.0030D 06	1.8870D 06	1.3920D-03	4.3590D-04
5.80	1.6910D 11	3.7570D 07	6.0160D 06	5.9280D 08	1.1860D 09	1.0030D 06	1.9310D 06	1.3980D-03	4.3710D-04
6.00	1.6380D 11	3.6430D 07	6.1290D 06	5.9310D 08	1.1850D 09	1.0030D 06	1.9750D 06	1.4020D-03	4.3830D-04
6.20	1.5880D 11	3.5340D 07	6.2390D 06	5.9320D 08	1.1850D 09	1.0030D 06	2.0190D 06	1.4060D-03	4.3950D-04
6.40	1.5410D 11	3.4300D 07	6.3460D 06	5.9310D 08	1.1840D 09	1.0040D 06	2.0630D 06	1.4100D-03	4.4060D-04
6.60	1.4970D 11	3.3310D 07	6.4490D 06	5.9290D 08	1.1840D 09	1.0040D 06	2.1070D 06	1.4130D-03	4.4170D-04
6.80	1.4550D 11	3.2360D 07	6.5500D 06	5.9260D 08	1.1830D 09	1.0040D 06	2.1510D 06	1.4150D-03	4.4270D-04
7.00	1.4150D 11	3.1450D 07	6.6470D 06	5.9200D 08	1.1830D 09	1.0040D 06	2.1950D 06	1.4170D-03	4.4370D-04
7.20	1.3770D 11	3.0580D 07	6.7410D 06	5.9140D 08	1.1820D 09	1.0040D 06	2.2390D 06	1.4190D-03	4.4470D-04
7.40	1.3410D 11	2.9740D 07	6.8330D 06	5.9070D 08	1.1820D 09	1.0040D 06	2.2820D 06	1.4200D-03	4.4570D-04
7.60	1.3060D 11	2.8940D 07	6.9220D 06	5.8980D 08	1.1810D 09	1.0040D 06	2.3260D 06	1.4210D-03	4.4660D-04
7.80	1.2730D 11	2.8170D 07	7.0090D 06	5.8890D 08	1.1810D 09	1.0040D 06	2.3700D 06	1.4210D-03	4.4750D-04
8.00	1.2420D 11	2.7440D 07	7.0930D 06	5.8780D 08	1.1800D 09	1.0040D 06	2.4130D 06	1.4210D-03	4.4830D-04
8.20	1.2120D 11	2.6730D 07	7.1740D 06	5.8670D 08	1.1800D 09	1.0040D 06	2.4560D 06	1.4210D-03	4.4910D-04
8.40	1.1830D 11	2.6040D 07	7.2530D 06	5.8540D 08	1.1790D 09	1.0040D 06	2.5000D 06	1.4210D-03	4.4990D-04
8.60	1.1560D 11	2.5390D 07	7.3300D 06	5.8410D 08	1.1790D 09	1.0040D 06	2.5430D 06	1.4200D-03	4.5070D-04
8.80	1.1290D 11	2.4760D 07	7.4050D 06	5.8280D 08	1.1780D 09	1.0040D 06	2.5860D 06	1.4190D-03	4.5140D-04
9.00	1.1040D 11	2.4150D 07	7.4780D 06	5.8130D 08	1.1780D 09	1.0040D 06	2.6290D 06	1.4180D-03	4.5210D-04
9.20	1.0800D 11	2.3560D 07	7.5490D 06	5.7980D 08	1.1770D 09	1.0040D 06	2.6720D 06	1.4160D-03	4.5280D-04
9.40	1.0570D 11	2.3000D 07	7.6180D 06	5.7830D 08	1.1770D 09	1.0040D 06	2.7140D 06	1.4140D-03	4.5350D-04
9.60	1.0340D 11	2.2450D 07	7.6840D 06	5.7670D 08	1.1770D 09	1.0040D 06	2.7570D 06	1.4130D-03	4.5410D-04
9.80	1.0130D 11	2.1930D 07	7.7500D 06	5.7500D 08	1.1760D 09	1.0040D 06	2.7990D 06	1.4100D-03	4.5470D-04
10.00	9.9180D 10	2.1420D 07	7.8130D 06	5.7330D 08	1.1760D 09	1.0040D 06	2.8420D 06	1.4080D-03	4.5530D-04

T= 800 K, H=30 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.27D 06	1.77D-15
2	2*NO3 >>> 2*NO2 + O2	3.98D-14	5.95D-48
3	NO2 + NO3 >>> NO2 + NO + O2	6.59D-14	3.13D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.74D-18
5	NO + O3 >>> NO2 + O2	3.43D-13	4.42D-26
6	NO2 + O3 >>> NO3 + O2	5.61D-15	9.78D-21
7	HNO3 + M >>> HO + NO2 + M	9.09D-01	2.01D-14
8	HNO3 + HO >>> H2O + NO3	9.00D-14	2.43D-18
9	O + O + M >>> O2 + M	3.39D-17	4.30D-17
10	O + O2 + M >>> O3 + M	2.12D-17	1.08D 01
11	O + O3 >>> 2*O2	1.07D-12	6.11D-39
12	O + NO + M >>> NO2 + M	3.40D-15	3.25D-09
13	O + NO2 >>> NO + O2	1.17D-11	5.55D-25
14	O + NO2 + M >>> NO3 + M	1.06D-14	8.47D-25
15	HO + HO >>> H2O + O	5.00D-12	1.06D-15
16	O2 + 2*NO >>> 2*NO2	6.40D-39	8.78D-20
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	9.55D-15
19	O + HO2 >>> HO + O2	4.28D-11	3.43D-26
20	O2 + H + M >>> HO2 + M	1.05D-15	1.57D-04
21	O3 + H >>> HO + O2	5.25D-11	6.31D-34
22	O3 + HO >>> HO2 + O2	4.30D-13	3.24D-24
23	O3 + HO2 >>> HO + 2*O2	1.48D-14	2.35D-48
24	H + HO + M >>> H2O + M	4.12D-15	4.08D-23
25	H + HO2 >>> 2*HO	1.28D-10	2.16D-22
26	H + HO2 >>> H2 + O2	2.71D-11	1.45D-26
27	H + H2O >>> H2 + HO	4.09D-16	1.41D-12
28	H + H2O2 >>> H2 + HO2	3.93D-13	9.47D-18
29	H + H2O2 >>> HO + H2O	5.11D-13	6.02D-33
30	2*HO + M >>> H2O2 + M	4.07D-15	3.36D-09
31	HO + HO2 >>> H2O + O2	4.44D-11	5.70D-30
32	2*HO2 >>> H2O2 + O2	9.10D-12	1.53D-22
33	HO2 + H2O >>> H2O2 + HO	5.19D-20	3.46D-17
34	NO + H + M >>> HNO + M	1.15D-15	6.86D-05
35	NO + HO >>> NO2 + H	3.30D-20	2.30D-10
36	NO + HO + M >>> HNO2 + M	1.64D-14	1.56D-01
37	NO + HO2 >>> NO2 + HO	4.46D-12	7.66D-14
38	H + H + M >>> H2 + M	1.06D-16	1.12D-21
39	HNO4 + M >>> HO2 + NO2 + M	1.76D 06	2.31D-15
40	CLNO3 + M >>> CLO + NO2 + M	1.16D 06	7.36D-16

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	4.0000D 08	4.2000D 09	3.0000D 06	4.5000D 08	2.5000D 12	7.8000D 16	4.0000D 08	3.0000D 06	1.2000D 12
0.20	2.5490D-04	4.4840D 08	4.0710D 08	6.3640D 09	3.9750D 11	7.8000D 16	3.3350D 08	1.8780D 09	1.2000D 12
0.40	3.3160D-05	5.9760D 07	3.9740D 08	6.8180D 09	2.3030D 11	7.8000D 16	2.7810D 08	2.6270D 09	1.1990D 12
0.60	2.6330D-05	4.8680D 07	3.8730D 08	6.8850D 09	2.0460D 11	7.8000D 16	2.3180D 08	3.3240D 09	1.1990D 12
0.80	2.5290D-05	4.7990D 07	3.7740D 08	6.9340D 09	1.8960D 11	7.8000D 16	1.9330D 08	3.9530D 09	1.1990D 12
1.00	2.4530D-05	4.7790D 07	3.6760D 08	6.9760D 09	1.7690D 11	7.8000D 16	1.6110D 08	4.5170D 09	1.1980D 12
1.20	2.3820D-05	4.7640D 07	3.5810D 08	7.0130D 09	1.6550D 11	7.8000D 16	1.3430D 08	5.0210D 09	1.1980D 12
1.40	2.3140D-05	4.7520D 07	3.4870D 08	7.0440D 09	1.5530D 11	7.8000D 16	1.1200D 08	5.4690D 09	1.1980D 12
1.60	2.2490D-05	4.7430D 07	3.3950D 08	7.0720D 09	1.4610D 11	7.8000D 16	9.3370D 07	5.8670D 09	1.1980D 12
1.80	2.1870D-05	4.7380D 07	3.3060D 08	7.0970D 09	1.3770D 11	7.8000D 16	7.7840D 07	6.2180D 09	1.1970D 12
2.00	2.1290D-05	4.7370D 07	3.2180D 08	7.1180D 09	1.3010D 11	7.8000D 16	6.4890D 07	6.5260D 09	1.1970D 12
2.20	2.0730D-05	4.7400D 07	3.1330D 08	7.1370D 09	1.2320D 11	7.8000D 16	5.4100D 07	6.7960D 09	1.1970D 12
2.40	2.0210D-05	4.7460D 07	3.0490D 08	7.1550D 09	1.1680D 11	7.8000D 16	4.5100D 07	7.0310D 09	1.1970D 12
2.60	1.9710D-05	4.7550D 07	2.9680D 08	7.1700D 09	1.1100D 11	7.8000D 16	3.7600D 07	7.2340D 09	1.1970D 12
2.80	1.9230D-05	4.7670D 07	2.8880D 08	7.1840D 09	1.0560D 11	7.8000D 16	3.1350D 07	7.4080D 09	1.1970D 12
3.00	1.8770D-05	4.7820D 07	2.8110D 08	7.1970D 09	1.0060D 11	7.8000D 16	2.6140D 07	7.5550D 09	1.1970D 12
3.20	1.8330D-05	4.7990D 07	2.7350D 08	7.2080D 09	9.6050D 10	7.8000D 16	2.1790D 07	7.6800D 09	1.1970D 12
3.40	1.7910D-05	4.8180D 07	2.6620D 08	7.2190D 09	9.1800D 10	7.8000D 16	1.8170D 07	7.7830D 09	1.1970D 12
3.60	1.7500D-05	4.8380D 07	2.5900D 08	7.2290D 09	8.7840D 10	7.8000D 16	1.5150D 07	7.8660D 09	1.1970D 12
3.80	1.7100D-05	4.8600D 07	2.5200D 08	7.2380D 09	8.4160D 10	7.8000D 16	1.2630D 07	7.9330D 09	1.1970D 12
4.00	1.6720D-05	4.8830D 07	2.4520D 08	7.2470D 09	8.0720D 10	7.8000D 16	1.0530D 07	7.9850D 09	1.1970D 12
4.20	1.6350D-05	4.9070D 07	2.3850D 08	7.2550D 09	7.7510D 10	7.8000D 16	8.7800D 06	8.0220D 09	1.1970D 12
4.40	1.5980D-05	4.9320D 07	2.3210D 08	7.2620D 09	7.4510D 10	7.8000D 16	7.3210D 06	8.0480D 09	1.1970D 12
4.60	1.5630D-05	4.9570D 07	2.2580D 08	7.2690D 09	7.1690D 10	7.8000D 16	6.1050D 06	8.0620D 09	1.1970D 12
4.80	1.5280D-05	4.9830D 07	2.1960D 08	7.2760D 09	6.9050D 10	7.8000D 16	5.0910D 06	8.0670D 09	1.1970D 12
5.00	1.4940D-05	5.0080D 07	2.1370D 08	7.2830D 09	6.6560D 10	7.8000D 16	4.2450D 06	8.0630D 09	1.1970D 12
5.20	1.4610D-05	5.0330D 07	2.0780D 08	7.2890D 09	6.4220D 10	7.8000D 16	3.5410D 06	8.0520D 09	1.1970D 12
5.40	1.4280D-05	5.0590D 07	2.0220D 08	7.2950D 09	6.2010D 10	7.8000D 16	2.9530D 06	8.0330D 09	1.1970D 12
5.60	1.3960D-05	5.0830D 07	1.9670D 08	7.3000D 09	5.9920D 10	7.8000D 16	2.4640D 06	8.0090D 09	1.1970D 12
5.80	1.3640D-05	5.1080D 07	1.9130D 08	7.3060D 09	5.7950D 10	7.8000D 16	2.0560D 06	7.9800D 09	1.1970D 12
6.00	1.3330D-05	5.1320D 07	1.8610D 08	7.3110D 09	5.6090D 10	7.8000D 16	1.7150D 06	7.9460D 09	1.1970D 12
6.20	1.3030D-05	5.1560D 07	1.8100D 08	7.3160D 09	5.4320D 10	7.8000D 16	1.4310D 06	7.9080D 09	1.1970D 12
6.40	1.2730D-05	5.1780D 07	1.7600D 08	7.3210D 09	5.2650D 10	7.8000D 16	1.1950D 06	7.8660D 09	1.1970D 12
6.60	1.2430D-05	5.2010D 07	1.7120D 08	7.3260D 09	5.1060D 10	7.8000D 16	9.9780D 05	7.8220D 09	1.1970D 12
6.80	1.2140D-05	5.2220D 07	1.6650D 08	7.3300D 09	4.9550D 10	7.8000D 16	8.3340D 05	7.7740D 09	1.1970D 12
7.00	1.1860D-05	5.2430D 07	1.6200D 08	7.3350D 09	4.8110D 10	7.8000D 16	6.9630D 05	7.7250D 09	1.1970D 12
7.20	1.1580D-05	5.2630D 07	1.5750D 08	7.3390D 09	4.6740D 10	7.8000D 16	5.8210D 05	7.6730D 09	1.1970D 12
7.40	1.1300D-05	5.2820D 07	1.5320D 08	7.3430D 09	4.5440D 10	7.8000D 16	4.8680D 05	7.6200D 09	1.1970D 12
7.60	1.1030D-05	5.3010D 07	1.4900D 08	7.3470D 09	4.4200D 10	7.8000D 16	4.0740D 05	7.5660D 09	1.1970D 12
7.80	1.0760D-05	5.3190D 07	1.4490D 08	7.3510D 09	4.3010D 10	7.8000D 16	3.4120D 05	7.5110D 09	1.1970D 12
8.00	1.0500D-05	5.3360D 07	1.4090D 08	7.3550D 09	4.1880D 10	7.8000D 16	2.8600D 05	7.4540D 09	1.1970D 12
8.20	1.0240D-05	5.3520D 07	1.3710D 08	7.3590D 09	4.0790D 10	7.8000D 16	2.3990D 05	7.3970D 09	1.1970D 12
8.40	9.9910D-06	5.3680D 07	1.3330D 08	7.3620D 09	3.9750D 10	7.8000D 16	2.0150D 05	7.3400D 09	1.1970D 12
8.60	9.7430D-06	5.3830D 07	1.2960D 08	7.3660D 09	3.8760D 10	7.8000D 16	1.6950D 05	7.2820D 09	1.1970D 12
8.80	9.4990D-06	5.3970D 07	1.2600D 08	7.3690D 09	3.7810D 10	7.8000D 16	1.4280D 05	7.2230D 09	1.1970D 12
9.00	9.2600D-06	5.4100D 07	1.2260D 08	7.3730D 09	3.6890D 10	7.8000D 16	1.2060D 05	7.1650D 09	1.1970D 12
9.20	9.0260D-06	5.4230D 07	1.1920D 08	7.3760D 09	3.6020D 10	7.8000D 16	1.0200D 05	7.1070D 09	1.1970D 12
9.40	8.7970D-06	5.4350D 07	1.1590D 08	7.3790D 09	3.5180D 10	7.8000D 16	8.6510D 04	7.0490D 09	1.1970D 12
9.60	8.5720D-06	5.4460D 07	1.1270D 08	7.3820D 09	3.4370D 10	7.8000D 16	7.3590D 04	6.9900D 09	1.1970D 12
9.80	8.3520D-06	5.4560D 07	1.0960D 08	7.3850D 09	3.3590D 10	7.8000D 16	6.2800D 04	6.9330D 09	1.1970D 12
10.00	8.1370D-06	5.4660D 07	1.0660D 08	7.3880D 09	3.2840D 10	7.8000D 16	5.3800D 04	6.8750D 09	1.1970D 12

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.000D 06	1.000D 06	1.000D 06	2.500D 07	1.200D 09	1.000D 06	0.000D 05	1.500D 09	2.000D 08
0.20	1.654D 12	1.534D 08	1.116D 06	1.774D 08	1.199D 09	1.000D 06	7.952D 05	1.041D-04	6.959D-05
0.40	1.612D 12	2.117D 08	1.369D 06	2.504D 08	1.196D 09	1.000D 06	8.195D 05	1.958D-05	9.275D-06
0.60	1.495D 12	2.474D 08	1.769D 06	3.186D 08	1.193D 09	1.001D 06	8.602D 05	2.030D-05	7.555D-06
0.80	1.369D 12	2.715D 08	2.312D 06	3.802D 08	1.189D 09	1.001D 06	9.150D 05	2.388D-05	7.448D-06
1.00	1.268D 12	2.875D 08	2.983D 06	4.354D 08	1.185D 09	1.002D 06	9.819D 05	2.723D-05	7.416D-06
1.20	1.178D 12	2.972D 08	3.765D 06	4.847D 08	1.181D 09	1.002D 06	1.059D 06	3.022D-05	7.393D-06
1.40	1.099D 12	3.022D 08	4.642D 06	5.286D 08	1.176D 09	1.002D 06	1.146D 06	3.287D-05	7.374D-06
1.60	1.028D 12	3.034D 08	5.592D 06	5.675D 08	1.171D 09	1.003D 06	1.240D 06	3.523D-05	7.361D-06
1.80	9.643D 11	3.019D 08	6.600D 06	6.018D 08	1.166D 09	1.003D 06	1.340D 06	3.732D-05	7.354D-06
2.00	9.070D 11	2.982D 08	7.649D 06	6.319D 08	1.161D 09	1.004D 06	1.444D 06	3.918D-05	7.352D-06
2.20	8.552D 11	2.929D 08	8.724D 06	6.583D 08	1.156D 09	1.004D 06	1.553D 06	4.083D-05	7.356D-06
2.40	8.081D 11	2.865D 08	9.814D 06	6.812D 08	1.150D 09	1.005D 06	1.665D 06	4.231D-05	7.365D-06
2.60	7.652D 11	2.792D 08	1.091D 07	7.009D 08	1.145D 09	1.005D 06	1.778D 06	4.362D-05	7.379D-06
2.80	7.260D 11	2.713D 08	1.199D 07	7.178D 08	1.139D 09	1.006D 06	1.893D 06	4.478D-05	7.398D-06
3.00	6.900D 11	2.631D 08	1.307D 07	7.321D 08	1.133D 09	1.006D 06	2.008D 06	4.581D-05	7.421D-06
3.20	6.568D 11	2.547D 08	1.412D 07	7.441D 08	1.127D 09	1.007D 06	2.123D 06	4.673D-05	7.447D-06
3.40	6.262D 11	2.461D 08	1.516D 07	7.540D 08	1.122D 09	1.007D 06	2.238D 06	4.754D-05	7.476D-06
3.60	5.980D 11	2.376D 08	1.616D 07	7.620D 08	1.116D 09	1.007D 06	2.351D 06	4.825D-05	7.508D-06
3.80	5.717D 11	2.292D 08	1.713D 07	7.683D 08	1.110D 09	1.008D 06	2.463D 06	4.887D-05	7.543D-06
4.00	5.474D 11	2.209D 08	1.808D 07	7.732D 08	1.104D 09	1.008D 06	2.573D 06	4.942D-05	7.579D-06
4.20	5.247D 11	2.128D 08	1.899D 07	7.767D 08	1.099D 09	1.008D 06	2.681D 06	4.988D-05	7.616D-06
4.40	5.036D 11	2.049D 08	1.986D 07	7.790D 08	1.093D 09	1.009D 06	2.787D 06	5.028D-05	7.654D-06
4.60	4.838D 11	1.972D 08	2.070D 07	7.802D 08	1.087D 09	1.009D 06	2.890D 06	5.062D-05	7.693D-06
4.80	4.653D 11	1.898D 08	2.151D 07	7.804D 08	1.082D 09	1.009D 06	2.990D 06	5.089D-05	7.732D-06
5.00	4.479D 11	1.827D 08	2.228D 07	7.799D 08	1.076D 09	1.010D 06	3.088D 06	5.111D-05	7.772D-06
5.20	4.317D 11	1.758D 08	2.302D 07	7.785D 08	1.070D 09	1.010D 06	3.182D 06	5.129D-05	7.811D-06
5.40	4.163D 11	1.692D 08	2.373D 07	7.766D 08	1.065D 09	1.010D 06	3.273D 06	5.141D-05	7.850D-06
5.60	4.019D 11	1.629D 08	2.440D 07	7.740D 08	1.059D 09	1.011D 06	3.361D 06	5.149D-05	7.889D-06
5.80	3.883D 11	1.568D 08	2.504D 07	7.709D 08	1.054D 09	1.011D 06	3.446D 06	5.154D-05	7.927D-06
6.00	3.755D 11	1.510D 08	2.565D 07	7.674D 08	1.048D 09	1.011D 06	3.528D 06	5.154D-05	7.964D-06
6.20	3.633D 11	1.454D 08	2.624D 07	7.635D 08	1.043D 09	1.011D 06	3.606D 06	5.152D-05	8.001D-06
6.40	3.518D 11	1.401D 08	2.679D 07	7.593D 08	1.038D 09	1.012D 06	3.682D 06	5.146D-05	8.036D-06
6.60	3.409D 11	1.350D 08	2.732D 07	7.547D 08	1.033D 09	1.012D 06	3.754D 06	5.137D-05	8.071D-06
6.80	3.306D 11	1.301D 08	2.783D 07	7.499D 08	1.027D 09	1.012D 06	3.822D 06	5.125D-05	8.104D-06
7.00	3.208D 11	1.255D 08	2.831D 07	7.449D 08	1.022D 09	1.012D 06	3.888D 06	5.111D-05	8.137D-06
7.20	3.114D 11	1.210D 08	2.876D 07	7.397D 08	1.017D 09	1.012D 06	3.951D 06	5.095D-05	8.168D-06
7.40	3.026D 11	1.168D 08	2.920D 07	7.344D 08	1.012D 09	1.013D 06	4.010D 06	5.077D-05	8.198D-06
7.60	2.941D 11	1.127D 08	2.961D 07	7.289D 08	1.007D 09	1.013D 06	4.067D 06	5.057D-05	8.227D-06
7.80	2.860D 11	1.088D 08	3.000D 07	7.233D 08	1.002D 09	1.013D 06	4.121D 06	5.035D-05	8.254D-06
8.00	2.783D 11	1.051D 08	3.037D 07	7.177D 08	9.972D 08	1.013D 06	4.171D 06	5.012D-05	8.281D-06
8.20	2.710D 11	1.016D 08	3.073D 07	7.120D 08	9.924D 08	1.013D 06	4.219D 06	4.987D-05	8.306D-06
8.40	2.640D 11	9.816D 07	3.107D 07	7.062D 08	9.876D 08	1.013D 06	4.264D 06	4.961D-05	8.330D-06
8.60	2.573D 11	9.492D 07	3.139D 07	7.004D 08	9.829D 08	1.014D 06	4.307D 06	4.934D-05	8.353D-06
8.80	2.508D 11	9.181D 07	3.169D 07	6.946D 08	9.782D 08	1.014D 06	4.347D 06	4.906D-05	8.375D-06
9.00	2.447D 11	8.884D 07	3.198D 07	6.888D 08	9.736D 08	1.014D 06	4.384D 06	4.877D-05	8.396D-06
9.20	2.388D 11	8.599D 07	3.226D 07	6.829D 08	9.690D 08	1.014D 06	4.419D 06	4.847D-05	8.415D-06
9.40	2.331D 11	8.324D 07	3.252D 07	6.771D 08	9.645D 08	1.014D 06	4.452D 06	4.816D-05	8.434D-06
9.60	2.277D 11	8.066D 07	3.277D 07	6.713D 08	9.600D 08	1.014D 06	4.482D 06	4.785D-05	8.451D-06
9.80	2.224D 11	7.815D 07	3.300D 07	6.656D 08	9.556D 08	1.014D 06	4.510D 06	4.753D-05	[illegible]
10.00	2.174D 11	7.576D 07	3.323D 07	6.598D 08	9.512D 08	1.014D 06	4.536D 06	4.721D-05	8.483D-06

T=250 K, H=35 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	9.80D-07	3.06D-14
2	2*NO3 >>> 2*NO2 + O2	4.71D-17	7.46D-62
3	NO2 + NO3 >>> NO2 + NO + O2	4.21D-15	1.19D-34
4	NO3 + NO >>> 2*NO2	1.90D-11	3.29D-32
5	NO + O3 >>> NO2 + O2	6.36D-15	1.08D-56
6	NO2 + O3 >>> NO3 + O2	6.65D-18	8.33D-39
7	HNO3 + M >>> HO + NO2 + M	1.30D-28	5.96D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.80D-29
9	O + O + M >>> O2 + M	6.52D-16	8.42D-59
10	O + O2 + M >>> O3 + M	1.40D-16	3.91D-13
11	O + O3 >>> 2*O2	1.92D-15	0.0
12	O + NO + M >>> NO2 + M	2.74D-14	2.03D-48
13	O + NO2 >>> NO + O2	5.12D-12	6.27D-53
14	O + NO2 + M >>> NO3 + M	1.71D-14	1.37D-24
15	HO + HO >>> H2O + O	1.09D-12	9.77D-27
16	O2 + 2*NO >>> 2*NO2	2.75D-38	3.88D-35
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	7.73D-25
19	O + HO2 >>> HO + O2	1.08D-11	5.45D-60
20	O2 + H + M >>> HO2 + M	6.74D-15	8.64D-32
21	O3 + H >>> HO + O2	1.27D-11	0.0
22	O3 + HO >>> HO2 + O2	2.75D-14	1.04D-48
23	O3 + HO2 >>> HO + 2*O2	4.45D-16	2.41D-68
24	H + HO + M >>> H2O + M	1.37D-13	0.0
25	H + HO2 >>> 2*HO	9.40D-12	1.62D-46
26	H + HO2 >>> H2 + O2	1.04D-11	2.55D-61
27	H + H2O >>> H2 + HO	2.34D-28	1.14D-15
28	H + H2O2 >>> H2 + HO2	8.36D-15	5.62D-29
29	H + H2O2 >>> HO + H2O	1.09D-14	1.35D-75
30	2*HO + M >>> H2O2 + M	7.83D-14	[illegible]
31	HO + HO2 >>> H2O + O2	1.12D-11	3.89D-74
32	2*HO2 >>> H2O2 + O2	2.30D-12	8.58D-49
33	HO2 + H2O >>> H2O2 + HO	1.02D-39	5.49D-13
34	NO + H + M >>> HNO + M	4.26D-15	6.67D-34
35	NO + HO >>> NO2 + H	3.05D-38	3.01D-11
36	NO + HO + M >>> HNO2 + M	5.60D-13	2.12D-26
37	NO + HO2 >>> NO2 + HO	1.65D-13	7.47D-21
38	H + H + M >>> H2 + M	1.71D-16	0.0
39	HNO4 + M >>> HO2 + NO2 + M	3.14D-06	5.80D-14
40	CLNO3 + M >>> CLO + NO2 + M	7.90D-08	4.32D-14

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	5.5000 07	2.2000 09	2.0000 06	5.5000 08	1.3000 12	3.8000 16	5.0000 07	5.0000 06	5.3000 11
0.20	5.5000 07	2.2010 09	2.0000 06	5.4910 08	1.3000 12	3.8000 16	5.0000 07	5.0250 06	5.3000 11
0.40	5.5000 07	2.2020 09	1.9990 06	5.4820 08	1.3000 12	3.8000 16	5.0000 07	4.9900 06	5.3000 11
0.60	5.5000 07	2.2030 09	1.9990 06	5.4730 08	1.3000 12	3.8000 16	5.0000 07	4.9550 06	5.3000 11
0.80	5.5000 07	2.2040 09	1.9990 06	5.4640 08	1.3000 12	3.8000 16	5.0010 07	4.9200 06	5.3000 11
1.00	5.5000 07	2.2050 09	1.9980 06	5.4550 08	1.3000 12	3.8000 16	5.0010 07	4.8850 06	5.3000 11
1.20	5.5000 07	2.2050 09	1.9980 06	5.4450 08	1.3000 12	3.8000 16	5.0010 07	4.8510 06	5.3000 11
1.40	5.5000 07	2.2060 09	1.9980 06	5.4360 08	1.3000 12	3.8000 16	5.0010 07	4.8170 06	5.3000 11
1.60	5.5000 07	2.2070 09	1.9970 06	5.4270 08	1.3000 12	3.8000 16	5.0010 07	4.7830 06	5.3000 11
1.80	5.5000 07	2.2080 09	1.9970 06	5.4180 08	1.3000 12	3.8000 16	5.0010 07	4.7500 06	5.3000 11
2.00	5.5000 07	2.2090 09	1.9970 06	5.4090 08	1.3000 12	3.8000 16	5.0010 07	4.7160 06	5.3000 11
2.20	5.5000 07	2.2100 09	1.9960 06	5.4000 08	1.3000 12	3.8000 16	5.0010 07	4.6830 06	5.3000 11
2.40	5.5000 07	2.2110 09	1.9960 06	5.3910 08	1.3000 12	3.8000 16	5.0020 07	4.6510 06	5.3000 11
2.60	5.5000 07	2.2120 09	1.9960 06	5.3820 08	1.3000 12	3.8000 16	5.0020 07	4.6180 06	5.3000 11
2.80	5.5000 07	2.2130 09	1.9950 06	5.3740 08	1.3000 12	3.8000 16	5.0020 07	4.5860 06	5.3000 11
3.00	5.5000 07	2.2130 09	1.9950 06	5.3650 08	1.3000 12	3.8000 16	5.0020 07	4.5540 06	5.3000 11
3.20	5.5000 07	2.2140 09	1.9950 06	5.3560 08	1.3000 12	3.8000 16	5.0020 07	4.5220 06	5.3000 11
3.40	5.5000 07	2.2150 09	1.9950 06	5.3470 08	1.3000 12	3.8000 16	5.0020 07	4.4910 06	5.3000 11
3.60	5.5000 07	2.2160 09	1.9940 06	5.3380 08	1.3000 12	3.8000 16	5.0020 07	4.4590 06	5.3000 11
3.80	5.5000 07	2.2170 09	1.9940 06	5.3290 08	1.3000 12	3.8000 16	5.0020 07	4.4280 06	5.3000 11
4.00	5.5000 07	2.2180 09	1.9940 06	5.3200 08	1.3000 12	3.8000 16	5.0020 07	4.3970 06	5.3000 11
4.20	5.5000 07	2.2190 09	1.9940 06	5.3110 08	1.3000 12	3.8000 16	5.0030 07	4.3670 06	5.3000 11
4.40	5.5000 07	2.2200 09	1.9940 06	5.3030 08	1.3000 12	3.8000 16	5.0030 07	4.3370 06	5.3000 11
4.60	5.5000 07	2.2210 09	1.9930 06	5.2940 08	1.3000 12	3.8000 16	5.0030 07	4.3060 06	5.3000 11
4.80	5.5000 07	2.2210 09	1.9930 06	5.2850 08	1.3000 12	3.8000 16	5.0030 07	4.2770 06	5.3000 11
5.00	5.5000 07	2.2220 09	1.9930 06	5.2760 08	1.3000 12	3.8000 16	5.0030 07	4.2470 06	5.3000 11
5.20	5.5000 07	2.2230 09	1.9930 06	5.2670 08	1.3000 12	3.8000 16	5.0030 07	4.2170 06	5.3000 11
5.40	5.5000 07	2.2240 09	1.9930 06	5.2590 08	1.3000 12	3.8000 16	5.0030 07	4.1880 06	5.3000 11
5.60	5.5000 07	2.2250 09	1.9930 06	5.2500 08	1.3000 12	3.8000 16	5.0030 07	4.1590 06	5.3000 11
5.80	5.5000 07	2.2260 09	1.9930 06	5.2410 08	1.3000 12	3.8000 16	5.0030 07	4.1310 06	5.3000 11
6.00	5.5000 07	2.2270 09	1.9920 06	5.2330 08	1.3000 12	3.8000 16	5.0040 07	4.1020 06	5.3000 11
6.20	5.5000 07	2.2280 09	1.9920 06	5.2240 08	1.3000 12	3.8000 16	5.0040 07	4.0740 06	5.3000 11
6.40	5.5000 07	2.2280 09	1.9920 06	5.2150 08	1.3000 12	3.8000 16	5.0040 07	4.0460 06	5.3000 11
6.60	5.5000 07	2.2290 09	1.9920 06	5.2070 08	1.3000 12	3.8000 16	5.0040 07	4.0180 06	5.3000 11
6.80	5.5000 07	2.2300 09	1.9920 06	5.1980 08	1.3000 12	3.8000 16	5.0040 07	3.9900 06	5.3000 11
7.00	5.5000 07	2.2310 09	1.9920 06	5.1890 08	1.3000 12	3.8000 16	5.0040 07	3.9620 06	5.3000 11
7.20	5.5000 07	2.2320 09	1.9920 06	5.1810 08	1.3000 12	3.8000 16	5.0040 07	3.9350 06	5.3000 11
7.40	5.5000 07	2.2330 09	1.9920 06	5.1720 08	1.3000 12	3.8000 16	5.0040 07	3.9080 06	5.3000 11
7.60	5.5000 07	2.2340 09	1.9920 06	5.1630 08	1.3000 12	3.8000 16	5.0040 07	3.8810 06	5.3000 11
7.80	5.5000 07	2.2340 09	1.9920 06	5.1550 08	1.3000 12	3.8000 16	5.0050 07	3.8550 06	5.3000 11
8.00	5.5000 07	2.2350 09	1.9920 06	5.1460 08	1.3000 12	3.8000 16	5.0050 07	3.8280 06	5.3000 11
8.20	5.5000 07	2.2360 09	1.9910 06	5.1380 08	1.3000 12	3.8000 16	5.0050 07	3.8020 06	5.3000 11
8.40	5.5000 07	2.2370 09	1.9910 06	5.1290 08	1.3000 12	3.8000 16	5.0050 07	3.7760 06	5.3000 11
8.60	5.5000 07	2.2380 09	1.9910 06	5.1210 08	1.3000 12	3.8000 16	5.0050 07	3.7500 06	5.3000 11
8.80	5.5000 07	2.2390 09	1.9910 06	5.1120 08	1.3000 12	3.8000 16	5.0050 07	3.7240 06	5.3000 11
9.00	5.5000 07	2.2400 09	1.9910 06	5.1040 08	1.3000 12	3.8000 16	5.0050 07	3.6990 06	5.3000 11
9.20	5.5000 07	2.2400 09	1.9910 06	5.0950 08	1.3000 12	3.8000 16	5.0050 07	3.6740 06	5.3000 11
9.40	5.5000 07	2.2410 09	1.9910 06	5.0870 08	1.3000 12	3.8000 16	5.0050 07	3.6490 06	5.3000 11
9.60	5.5000 07	2.2420 09	1.9910 06	5.0780 08	1.3000 12	3.8000 16	5.0050 07	3.6240 06	5.3000 11
9.80	5.5000 07	2.2430 09	1.9910 06	5.0700 08	1.3000 12	3.8000 16	5.0060 07	3.5990 06	5.3000 11
10.00	5.5000 07	2.2440 09	1.9910 06	5.0620 08	1.3000 12	3.8000 16	5.0060 07	3.5750 06	5.3000 11

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000 06	1.0000 06	1.0000 06	1.7000 07	2.8000 08	1.0000 06	7.0000 05	2.3000 08	4.0000 07
0.20	3.4530 05	2.7240-01	1.0000 06	1.7970 07	2.8000 08	1.0000 06	7.0030 05	2.3000 08	4.0000 07
0.40	1.1920 05	9.3470-02	1.0000 06	1.8010 07	2.8000 08	1.0000 06	7.0060 05	2.3000 08	4.0000 07
0.60	4.1170 04	3.2060-02	1.0000 06	1.8040 07	2.8000 08	1.0000 06	7.0090 05	2.3000 08	4.0000 07
0.80	1.4220 04	1.1010-02	1.0000 06	1.8070 07	2.8000 08	1.0000 06	7.0120 05	2.3000 08	4.0000 07
1.00	4.9120 03	3.7900-03	1.0000 06	1.8100 07	2.8000 08	1.0000 06	7.0150 05	2.3000 08	4.0000 07
1.20	1.6990 03	1.3150-03	1.0000 06	1.8130 07	2.8000 08	1.0000 06	7.0180 05	2.3000 08	4.0010 07
1.40	5.8980 02	4.6640-04	1.0000 06	1.8160 07	2.8000 08	1.0000 06	7.0210 05	2.3000 08	4.0010 07
1.60	2.0680 02	1.7530-04	1.0000 06	1.8200 07	2.8000 08	1.0000 06	7.0240 05	2.3000 08	4.0010 07
1.80	7.4500 01	7.5380-05	1.0000 06	1.8230 07	2.8000 08	1.0000 06	7.0270 05	2.3000 08	4.0010 07
2.00	2.8780 01	4.0980-05	1.0000 06	1.8260 07	2.8000 08	1.0000 06	7.0300 05	2.3000 08	4.0010 07
2.20	1.2950 01	2.9050-05	1.0000 06	1.8290 07	2.8000 08	1.0000 06	7.0330 05	2.3000 08	4.0010 07
2.40	7.4430 00	2.4820-05	1.0000 06	1.8320 07	2.8000 08	1.0000 06	7.0360 05	2.3000 08	4.0010 07
2.60	5.5010 00	2.3240-05	1.0000 06	1.8350 07	2.8000 08	1.0000 06	7.0380 05	2.3000 08	4.0010 07
2.80	4.7910 00	2.2570-05	1.0000 06	1.8380 07	2.8000 08	1.0000 06	7.0410 05	2.3000 08	4.0010 07
3.00	4.5060 00	2.2210-05	1.0000 06	1.8410 07	2.8000 08	1.0000 06	7.0440 05	2.3000 08	4.0010 07
3.20	4.3690 00	2.1960-05	1.0000 06	1.8440 07	2.8000 08	1.0000 06	7.0470 05	2.3000 08	4.0020 07
3.40	4.2840 00	2.1740-05	1.0000 06	1.8470 07	2.8000 08	1.0000 06	7.0490 05	2.3000 08	4.0020 07
3.60	4.2170 00	2.1550-05	1.0000 06	1.8490 07	2.8000 08	1.0000 06	7.0520 05	2.3000 08	4.0020 07
3.80	4.1560 00	2.1360-05	1.0000 06	1.8520 07	2.8000 08	1.0000 06	7.0550 05	2.3000 08	4.0020 07
4.00	4.0990 00	2.1170-05	1.0000 06	1.8550 07	2.8000 08	1.0000 06	7.0570 05	2.3000 08	4.0020 07
4.20	4.0430 00	2.0980-05	1.0000 06	1.8580 07	2.8000 08	1.0000 06	7.0600 05	2.3000 08	4.0020 07
4.40	3.9880 00	2.0800-05	1.0000 06	1.8610 07	2.8000 08	1.0000 06	7.0620 05	2.3000 08	4.0020 07
4.60	3.9340 00	2.0620-05	1.0000 06	1.8640 07	2.8000 08	1.0000 06	7.0650 05	2.3000 08	4.0020 07
4.80	3.8810 00	2.0440-05	1.0000 06	1.8660 07	2.8000 08	1.0000 06	7.0680 05	2.3000 08	4.0020 07
5.00	3.8290 00	2.0270-05	1.0000 06	1.8690 07	2.8000 08	1.0000 06	7.0700 05	2.3000 08	4.0020 07
5.20	3.7770 00	2.0090-05	1.0000 06	1.8720 07	2.8000 08	1.0000 06	7.0730 05	2.3000 08	4.0020 07
5.40	3.7260 00	1.9920-05	1.0000 06	1.8740 07	2.8000 08	1.0000 06	7.0750 05	2.3000 08	4.0030 07
5.60	3.6760 00	1.9750-05	1.0000 06	1.8770 07	2.8000 08	1.0000 06	7.0780 05	2.3000 08	4.0030 07
5.80	3.6270 00	1.9580-05	1.0000 06	1.8800 07	2.8000 08	1.0000 06	7.0800 05	2.3000 08	4.0030 07
6.00	3.5780 00	1.9420-05	1.0000 06	1.8820 07	2.8000 08	1.0000 06	7.0820 05	2.3000 08	4.0030 07
6.20	3.5300 00	1.9250-05	1.0000 06	1.8850 07	2.8000 08	1.0000 06	7.0850 05	2.3000 08	4.0030 07
6.40	3.4830 00	1.9090-05	1.0000 06	1.8870 07	2.8000 08	1.0000 06	7.0870 05	2.3000 08	4.0030 07
6.60	3.4360 00	1.8930-05	1.0000 06	1.8900 07	2.8000 08	1.0000 06	7.0890 05	2.3000 08	4.0030 07
6.80	3.3900 00	1.8770-05	1.0000 06	1.8930 07	2.8000 08	1.0000 06	7.0920 05	2.3000 08	4.0030 07
7.00	3.3450 00	1.8610-05	1.0000 06	1.8950 07	2.8000 08	1.0000 06	7.0940 05	2.3000 08	4.0030 07
7.20	3.3000 00	1.8460-05	1.0000 06	1.8980 07	2.8000 08	1.0000 06	7.0960 05	2.3000 08	4.0030 07
7.40	3.2560 00	1.8300-05	1.0000 06	1.9000 07	2.8000 08	1.0000 06	7.0990 05	2.3000 08	4.0040 07
7.60	3.2130 00	1.8150-05	1.0000 06	1.9030 07	2.8000 08	1.0000 06	7.1010 05	2.3000 08	4.0040 07
7.80	3.1700 00	1.8000-05	1.0000 06	1.9050 07	2.8000 08	1.0000 06	7.1030 05	2.3000 08	4.0040 07
8.00	3.1280 00	1.7850-05	1.0000 06	1.9070 07	2.8000 08	1.0000 06	7.1050 05	2.3000 08	4.0040 07
8.20	3.0870 00	1.7710-05	1.0000 06	1.9100 07	2.8000 08	1.0000 06	7.1080 05	2.3000 08	4.0040 07
8.40	3.0460 00	1.7560-05	1.0000 06	1.9120 07	2.8000 08	1.0000 06	7.1100 05	2.3000 08	4.0040 07
8.60	3.0060 00	1.7420-05	1.0000 06	1.9150 07	2.8000 08	1.0000 06	7.1120 05	2.3000 08	4.0040 07
8.80	2.9660 00	1.7280-05	1.0000 06	1.9170 07	2.8000 08	1.0000 06	7.1140 05	2.3000 08	4.0040 07
9.00	2.9270 00	1.7140-05	1.0000 06	1.9190 07	2.8000 08	1.0000 06	7.1160 05	2.3000 08	4.0040 07
9.20	2.8880 00	1.7000-05	1.0000 06	1.9210 07	2.8000 08	1.0000 06	7.1180 05	2.3000 08	4.0040 07
9.40	2.8500 00	1.6860-05	1.0000 06	1.9240 07	2.8000 08	1.0000 06	7.1200 05	2.3000 08	4.0040 07
9.60	2.8130 00	1.6730-05	1.0000 06	1.9260 07	2.8000 08	1.0000 06	7.1220 05	2.3000 08	4.0050 07
9.80	2.7760 00	1.6590-05	1.0000 06	1.9280 07	2.8000 08	1.0000 06	7.1250 05	2.3000 08	4.0050 07
10.00	2.7390 00	1.6460-05	1.0000 06	1.9310 07	2.8000 08	1.0000 06	7.1270 05	2.3000 08	4.0050 07

T=300 K, H=35 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	7.93D-04	1.44D-14
2	2*NO3 >>> 2*NO2 + O2	2.41D-16	1.75D-58
3	NO2 + NO3 >>> NO2 + NO + O2	8.21D-15	4.92D-35
4	NO3 + NO >>> 2*NO2	1.90D-11	6.98D-29
5	NO + O3 >>> NO2 + O2	1.67D-14	2.85D-49
6	NO2 + O3 >>> NO3 + O2	3.41D-17	2.00D-34
7	HNO3 + M >>> HO + NO2 + M	9.70D-22	3.15D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	1.25D-26
9	O + O + M >>> O2 + M	2.98D-16	3.21D-59
10	O + O2 + M >>> O3 + M	8.28D-17	6.65D-10
11	O + O3 >>> 2*O2	8.90D-15	0.0
12	O + NO + M >>> NO2 + M	1.55D-14	6.07D-39
13	O + NO2 >>> NO + O2	6.25D-12	3.73D-46
14	O + NO2 + M >>> NO3 + M	1.43D-14	1.14D-24
15	HO + HO >>> H2O + O	1.57D-12	4.63D-24
16	O2 + 2*NO >>> 2*NO2	1.93D-38	2.26D-31
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.16D-22
19	O + HO2 >>> HO + O2	1.51D-11	8.51D-52
20	O2 + H + M >>> HO2 + M	4.03D-15	3.28D-25
21	O3 + H >>> HO + O2	1.79D-11	1.62D-69
22	O3 + HO >>> HO2 + O2	5.35D-14	8.98D-43
23	O3 + HO2 >>> HO + 2*O2	1.04D-15	1.53D-63
24	H + HO + M >>> H2O + M	7.12D-14	5.77D-76
25	H + HO2 >>> 2*HO	1.77D-11	1.14D-40
26	H + HO2 >>> H2 + O2	1.31D-11	6.80D-53
27	H + H2O >>> H2 + HO	2.18D-25	6.41D-15
28	H + H2O2 >>> H2 + HO2	2.13D-14	2.96D-26
29	H + H2O2 >>> HO + H2O	2.76D-14	2.95D-65
30	2*HO + M >>> H2O2 + M	3.58D-14	2.61D-25
31	HO + HO2 >>> H2O + O2	1.57D-11	1.98D-63
32	2*HO2 >>> H2O2 + O2	3.21D-12	1.98D-42
33	HO2 + H2O >>> H2O2 + HO	6.11D-35	8.57D-13
34	NO + H + M >>> HNO + M	2.91D-15	7.45D-27
35	NO + HO >>> NO2 + H	7.19D-34	4.92D-11
36	NO + HO + M >>> HNO2 + M	2.23D-13	1.25D-22
37	NO + HO2 >>> NO2 + HO	3.66D-13	3.74D-19
38	H + H + M >>> H2 + M	1.43D-16	1.23D-69
39	HNO4 + M >>> HO2 + NO2 + M	2.09D-03	2.50D-14
40	CLNO3 + M >>> CLO + NO2 + M	1.15D-04	2.07D-14

AD-A085 198 PERKIN-ELMER CORP NORWALK CONN ELECTRO-OPTICAL DIV F/G 13/2
HIGH ALTITUDE POLLUTION PROGRAM STRATOSPHERIC MEASUREMENT SYSTE--ETC(U)
FEB 80 N H MACOY, R WEINGARTEN, A PIRES DOT-FA77WA-4080
UNCLASSIFIED PE-14262 FAA/EE-80-11 NL

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A085 198

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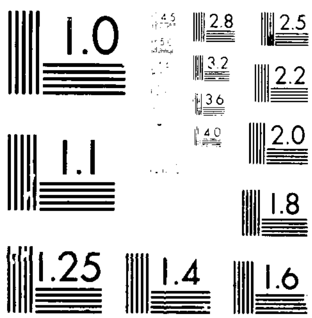

MICROCOPY RESOLUTION TEST CHART

NATIONAL BUREAU OF STANDARDS-1963-A

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	5.5000D 07	2.2000D 09	2.0000 06	5.5000D 08	1.3000D 12	3.8000D 16	5.0000D 07	5.0000 06	5.3000 11
0.20	5.4990D 07	2.2020D 09	2.0240D 06	5.4760D 08	1.3000D 12	3.8000D 16	5.0000D 07	5.0660D 06	5.3000 11
0.40	5.4980D 07	2.2050D 09	2.0480D 06	5.4520D 08	1.3000D 12	3.8000D 16	5.0000D 07	5.0000D 06	5.3000D 11
0.60	5.4970D 07	2.2070D 09	2.0720D 06	5.4290D 08	1.3000D 12	3.8000D 16	5.0000D 07	4.9350D 06	5.3000D 11
0.80	5.4970D 07	2.2100D 09	2.0960D 06	5.4050D 08	1.3000D 12	3.8000D 16	5.0000D 07	4.8720D 06	5.3000D 11
1.00	5.4960D 07	2.2120D 09	2.1200D 06	5.3820D 08	1.3000D 12	3.8000D 16	5.0000D 07	4.8090D 06	5.3000D 11
1.20	5.4950D 07	2.2150D 09	2.1440D 06	5.3580D 08	1.3000D 12	3.8000D 16	5.0000D 07	4.7470D 06	5.3000D 11
1.40	5.4940D 07	2.2170D 09	2.1680D 06	5.3350D 08	1.3000D 12	3.8000D 16	5.0000D 07	4.6860D 06	5.3000D 11
1.60	5.4930D 07	2.2200D 09	2.1920D 06	5.3120D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.6260D 06	5.3000D 11
1.80	5.4920D 07	2.2220D 09	2.2160D 06	5.2890D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.5660D 06	5.3000D 11
2.00	5.4910D 07	2.2240D 09	2.2400D 06	5.2660D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.5080D 06	5.3000D 11
2.20	5.4900D 07	2.2270D 09	2.2640D 06	5.2430D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.4500D 06	5.3000D 11
2.40	5.4900D 07	2.2290D 09	2.2870D 06	5.2200D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.3940D 06	5.3000D 11
2.60	5.4890D 07	2.2310D 09	2.3110D 06	5.1970D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.3380D 06	5.3000D 11
2.80	5.4880D 07	2.2340D 09	2.3350D 06	5.1750D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.2830D 06	5.3000D 11
3.00	5.4870D 07	2.2360D 09	2.3590D 06	5.1520D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.2290D 06	5.3000D 11
3.20	5.4860D 07	2.2380D 09	2.3830D 06	5.1300D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.1750D 06	5.3000D 11
3.40	5.4850D 07	2.2410D 09	2.4070D 06	5.1070D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.1230D 06	5.3000D 11
3.60	5.4840D 07	2.2430D 09	2.4310D 06	5.0850D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.0710D 06	5.3000D 11
3.80	5.4830D 07	2.2450D 09	2.4540D 06	5.0630D 08	1.3000D 12	3.8000D 16	5.0010D 07	4.0200D 06	5.3000D 11
4.00	5.4830D 07	2.2480D 09	2.4780D 06	5.0410D 08	1.3000D 12	3.8000D 16	5.0010D 07	3.9700D 06	5.3000D 11
4.20	5.4820D 07	2.2500D 09	2.5020D 06	5.0190D 08	1.3000D 12	3.8000D 16	5.0010D 07	3.9200D 06	5.3000D 11
4.40	5.4810D 07	2.2520D 09	2.5260D 06	4.9970D 08	1.3000D 12	3.8000D 16	5.0010D 07	3.8710D 06	5.3000D 11
4.60	5.4800D 07	2.2540D 09	2.5500D 06	4.9760D 08	1.3000D 12	3.8000D 16	5.0010D 07	3.8230D 06	5.3000D 11
4.80	5.4790D 07	2.2570D 09	2.5740D 06	4.9540D 08	1.3000D 12	3.8000D 16	5.0010D 07	3.7760D 06	5.3000D 11
5.00	5.4780D 07	2.2590D 09	2.5970D 06	4.9330D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.7290D 06	5.3000D 11
5.20	5.4770D 07	2.2610D 09	2.6210D 06	4.9110D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.6830D 06	5.3000D 11
5.40	5.4770D 07	2.2630D 09	2.6450D 06	4.8900D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.6380D 06	5.3000D 11
5.60	5.4760D 07	2.2660D 09	2.6690D 06	4.8680D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.5930D 06	5.3000D 11
5.80	5.4750D 07	2.2680D 09	2.6930D 06	4.8470D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.5490D 06	5.3000D 11
6.00	5.4740D 07	2.2700D 09	2.7160D 06	4.8260D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.5060D 06	5.3000D 11
6.20	5.4730D 07	2.2720D 09	2.7400D 06	4.8050D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.4630D 06	5.3000D 11
6.40	5.4720D 07	2.2740D 09	2.7640D 06	4.7840D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.4210D 06	5.3000D 11
6.60	5.4710D 07	2.2770D 09	2.7880D 06	4.7640D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.3800D 06	5.3000D 11
6.80	5.4700D 07	2.2790D 09	2.8110D 06	4.7430D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.3390D 06	5.3000D 11
7.00	5.4700D 07	2.2810D 09	2.8350D 06	4.7220D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.2990D 06	5.3000D 11
7.20	5.4690D 07	2.2830D 09	2.8590D 06	4.7020D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.2600D 06	5.3000D 11
7.40	5.4680D 07	2.2850D 09	2.8830D 06	4.6810D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.2210D 06	5.3000D 11
7.60	5.4670D 07	2.2870D 09	2.9060D 06	4.6610D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.1820D 06	5.3000D 11
7.80	5.4660D 07	2.2890D 09	2.9300D 06	4.6410D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.1450D 06	5.3000D 11
8.00	5.4650D 07	2.2910D 09	2.9540D 06	4.6200D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.1070D 06	5.3000D 11
8.20	5.4640D 07	2.2940D 09	2.9780D 06	4.6000D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.0710D 06	5.3000D 11
8.40	5.4640D 07	2.2960D 09	3.0010D 06	4.5800D 08	1.3000D 12	3.8000D 16	5.0020D 07	3.0350D 06	5.3000D 11
8.60	5.4630D 07	2.2980D 09	3.0250D 06	4.5600D 08	1.3000D 12	3.8000D 16	5.0020D 07	2.9990D 06	5.3000D 11
8.80	5.4620D 07	2.3000D 09	3.0490D 06	4.5410D 08	1.3000D 12	3.8000D 16	5.0020D 07	2.9640D 06	5.3000D 11
9.00	5.4610D 07	2.3020D 09	3.0730D 06	4.5210D 08	1.3000D 12	3.8000D 16	5.0020D 07	2.9300D 06	5.3000D 11
9.20	5.4600D 07	2.3040D 09	3.0960D 06	4.5010D 08	1.3000D 12	3.8000D 16	5.0030D 07	2.8960D 06	5.3000D 11
9.40	5.4590D 07	2.3060D 09	3.1200D 06	4.4820D 08	1.3000D 12	3.8000D 16	5.0030D 07	2.8620D 06	5.3000D 11
9.60	5.4580D 07	2.3080D 09	3.1440D 06	4.4620D 08	1.3000D 12	3.8000D 16	5.0030D 07	2.8290D 06	5.3000D 11
9.80	5.4580D 07	2.3100D 09	3.1680D 06	4.4430D 08	1.3000D 12	3.8000D 16	5.0030D 07	2.7970D 06	5.3000D 11
10.00	5.4570D 07	2.3120D 09	3.1910D 06	4.4230D 08	1.3000D 12	3.8000D 16	5.0030D 07	2.7650D 06	5.3000D 11

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	1.7000D 07	2.8000D 08	1.0000D 06	7.0000D 05	2.3000D 08	4.0000D 07
0.20	5.3050D 05	6.5250D-01	1.0000D 06	1.8030D 07	2.8000D 08	1.0000D 06	7.0010D 05	2.2990D 08	4.0000D 07
0.40	2.8150D 05	3.4180D-01	1.0000D 06	1.8190D 07	2.8000D 08	1.0000D 06	7.0020D 05	2.2980D 08	4.0000D 07
0.60	1.4940D 05	1.7920D-01	1.0000D 06	1.8350D 07	2.8000D 08	1.0000D 06	7.0040D 05	2.2970D 08	4.0000D 07
0.80	7.9370D 04	9.4030D-02	1.0000D 06	1.8500D 07	2.8000D 08	1.0000D 06	7.0050D 05	2.2960D 08	4.0000D 07
1.00	4.2220D 04	4.9460D-02	1.0000D 06	1.8660D 07	2.8000D 08	1.0000D 06	7.0060D 05	2.2950D 08	4.0000D 07
1.20	2.2530D 04	2.6120D-02	1.0000D 06	1.8820D 07	2.8000D 08	1.0000D 06	7.0070D 05	2.2940D 08	4.0000D 07
1.40	1.2080D 04	1.3900D-02	1.0000D 06	1.8970D 07	2.8000D 08	1.0000D 06	7.0080D 05	2.2930D 08	4.0000D 07
1.60	6.5390D 03	7.5050D-03	1.0000D 06	1.9130D 07	2.8000D 08	1.0000D 06	7.0090D 05	2.2920D 08	4.0000D 07
1.80	3.6010D 03	4.1520D-03	1.0000D 06	1.9280D 07	2.8000D 08	1.0000D 06	7.0100D 05	2.2910D 08	4.0000D 07
2.00	2.0420D 03	2.3930D-03	1.0000D 06	1.9430D 07	2.8000D 08	1.0000D 06	7.0120D 05	2.2900D 08	4.0000D 07
2.20	1.2160D 03	1.4700D-03	1.0000D 06	1.9580D 07	2.8000D 08	1.0000D 06	7.0130D 05	2.2890D 08	3.9990D 07
2.40	7.7720D 02	9.8340D-04	1.0000D 06	1.9730D 07	2.8000D 08	1.0000D 06	7.0140D 05	2.2890D 08	3.9990D 07
2.60	5.4450D 02	7.2590D-04	1.0000D 06	1.9880D 07	2.8000D 08	1.0000D 06	7.0150D 05	2.2880D 08	3.9990D 07
2.80	4.2100D 02	5.8830D-04	1.0000D 06	2.0030D 07	2.8000D 08	1.0000D 06	7.0160D 05	2.2870D 08	3.9990D 07
3.00	3.5540D 02	5.1350D-04	1.0000D 06	2.0180D 07	2.8000D 08	1.0000D 06	7.0170D 05	2.2860D 08	3.9990D 07
3.20	3.2050D 02	4.7170D-04	1.0000D 06	2.0320D 07	2.8000D 08	1.0000D 06	7.0180D 05	2.2850D 08	3.9990D 07
3.40	3.0190D 02	4.4710D-04	1.0000D 06	2.0470D 07	2.8000D 08	1.0000D 06	7.0190D 05	2.2840D 08	3.9990D 07
3.60	2.9190D 02	4.3160D-04	1.0000D 06	2.0610D 07	2.8000D 08	1.0000D 06	7.0190D 05	2.2830D 08	3.9990D 07
3.80	2.8660D 02	4.2190D-04	1.0000D 06	2.0760D 07	2.8000D 08	1.0000D 06	7.0200D 05	2.2820D 08	3.9990D 07
4.00	2.8360D 02	4.1290D-04	1.0000D 06	2.0900D 07	2.8000D 08	1.0000D 06	7.0210D 05	2.2810D 08	3.9990D 07
4.20	2.8200D 02	4.0610D-04	1.0000D 06	2.1040D 07	2.8000D 08	1.0000D 06	7.0220D 05	2.2800D 08	3.9990D 07
4.40	2.8100D 02	4.0020D-04	1.0000D 06	2.1190D 07	2.8000D 08	1.0000D 06	7.0230D 05	2.2790D 08	3.9990D 07
4.60	2.8040D 02	3.9460D-04	1.0000D 06	2.1330D 07	2.8000D 08	1.0000D 06	7.0240D 05	2.2780D 08	3.9990D 07
4.80	2.8000D 02	3.8940D-04	1.0000D 06	2.1470D 07	2.8000D 08	1.0000D 06	7.0250D 05	2.2770D 08	3.9990D 07
5.00	2.7970D 02	3.8430D-04	1.0000D 06	2.1610D 07	2.8000D 08	1.0000D 06	7.0260D 05	2.2760D 08	3.9990D 07
5.20	2.7940D 02	3.7940D-04	1.0000D 06	2.1750D 07	2.8000D 08	1.0000D 06	7.0260D 05	2.2750D 08	3.9990D 07
5.40	2.7920D 02	3.7450D-04	1.0000D 06	2.1880D 07	2.8000D 08	1.0000D 06	7.0270D 05	2.2740D 08	3.9990D 07
5.60	2.7900D 02	3.6980D-04	1.0000D 06	2.2020D 07	2.8000D 08	1.0000D 06	7.0280D 05	2.2730D 08	3.9990D 07
5.80	2.7890D 02	3.6510D-04	1.0000D 06	2.2160D 07	2.8000D 08	1.0000D 06	7.0290D 05	2.2720D 08	3.9990D 07
6.00	2.7870D 02	3.6050D-04	1.0000D 06	2.2300D 07	2.8000D 08	1.0000D 06	7.0290D 05	2.2710D 08	3.9990D 07
6.20	2.7850D 02	3.5600D-04	1.0000D 06	2.2430D 07	2.8000D 08	1.0000D 06	7.0300D 05	2.2710D 08	3.9990D 07
6.40	2.7840D 02	3.5150D-04	1.0000D 06	2.2570D 07	2.8000D 08	1.0000D 06	7.0310D 05	2.2700D 08	3.9990D 07
6.60	2.7820D 02	3.4720D-04	1.0000D 06	2.2700D 07	2.8000D 08	1.0000D 06	7.0320D 05	2.2690D 08	3.9980D 07
6.80	2.7810D 02	3.4290D-04	1.0000D 06	2.2830D 07	2.8000D 08	1.0000D 06	7.0320D 05	2.2680D 08	3.9980D 07
7.00	2.7800D 02	3.3860D-04	1.0000D 06	2.2970D 07	2.8000D 08	1.0000D 06	7.0330D 05	2.2670D 08	3.9980D 07
7.20	2.7780D 02	3.3450D-04	1.0000D 06	2.3100D 07	2.8000D 08	1.0000D 06	7.0340D 05	2.2660D 08	3.9980D 07
7.40	2.7770D 02	3.3040D-04	1.0000D 06	2.3230D 07	2.8000D 08	1.0000D 06	7.0340D 05	2.2650D 08	3.9980D 07
7.60	2.7760D 02	3.2640D-04	1.0000D 06	2.3360D 07	2.8000D 08	1.0000D 06	7.0350D 05	2.2640D 08	3.9980D 07
7.80	2.7740D 02	3.2240D-04	1.0000D 06	2.3490D 07	2.8000D 08	1.0000D 06	7.0360D 05	2.2630D 08	3.9980D 07
8.00	2.7730D 02	3.1850D-04	1.0000D 06	2.3620D 07	2.8000D 08	1.0000D 06	7.0360D 05	2.2620D 08	3.9980D 07
8.20	2.7720D 02	3.1460D-04	1.0000D 06	2.3750D 07	2.8000D 08	1.0000D 06	7.0370D 05	2.2610D 08	3.9980D 07
8.40	2.7710D 02	3.1080D-04	1.0000D 06	2.3880D 07	2.8000D 08	1.0000D 06	7.0380D 05	2.2600D 08	3.9980D 07
8.60	2.7700D 02	3.0710D-04	1.0000D 06	2.4010D 07	2.8000D 08	1.0000D 06	7.0380D 05	2.2590D 08	3.9980D 07
8.80	2.7690D 02	3.0350D-04	1.0000D 06	2.4130D 07	2.8000D 08	1.0000D 06	7.0390D 05	2.2580D 08	3.9980D 07
9.00	2.7680D 02	2.9990D-04	1.0000D 06	2.4260D 07	2.8000D 08	1.0000D 06	7.0390D 05	2.2570D 08	3.9980D 07
9.20	2.7670D 02	2.9630D-04	1.0000D 06	2.4390D 07	2.8000D 08	1.0000D 06	7.0400D 05	2.2560D 08	3.9980D 07
9.40	2.7650D 02	2.9280D-04	1.0000D 06	2.4510D 07	2.8000D 08	1.0000D 06	7.0410D 05	2.2550D 08	3.9980D 07
9.60	2.7650D 02	2.8940D-04	1.0000D 06	2.4640D 07	2.8000D 08	1.0000D 06	7.0410D 05	2.2550D 08	3.9980D 07
9.80	2.7640D 02	2.8600D-04	1.0000D 06	2.4760D 07	2.8000D 08	1.0000D 06	7.0420D 05	2.2540D 08	3.9980D 07
10.00	2.7630D 02	2.8270D-04	1.0000D 06	2.4880D 07	2.8000D 08	1.0000D 06	7.0420D 05	2.2530D 08	3.9980D 07

T=700 K, H=35 km

R NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	1.16D 05	1.20D-14
2	2*NO3 >>> 2*NO2 + O2	2.57D-14	7.44D-49
3	NO2 + NO3 >>> NO2 + NO + O2	5.51D-14	3.97D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.23D-19
5	NO + O3 >>> NO2 + O2	2.65D-13	4.54D-28
6	NO2 + O3 >>> NO3 + O2	3.62D-15	6.56D-22
7	HNO3 + M >>> HO + NO2 + M	9.70D-03	1.62D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	4.74D-19
9	O + O + M >>> O2 + M	2.30D-17	3.64D-22
10	O + O2 + M >>> O3 + M	1.34D-17	8.12D-01
11	O + O3 >>> 2*O2	7.11D-13	8.63D-43
12	O + NO + M >>> NO2 + M	2.18D-15	5.17D-12
13	O + NO2 >>> NO + O2	1.11D-11	8.50D-27
14	O + NO2 + M >>> NO3 + M	6.11D-15	4.89D-25
15	HO + HO >>> H2O + O	4.53D-12	2.04D-16
16	O2 + 2*NO >>> 2*NO2	7.04D-39	9.37D-21
17	NO2 + H-NO >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	2.11D-15
19	O + HO2 >>> HO + O2	3.91D-11	2.19D-28
20	O2 + H + M >>> HO2 + M	6.66D-16	1.50D-06
21	O3 + H >>> HO + O2	4.78D-11	5.62D-37
22	O3 + HO >>> HO2 + O2	3.59D-13	8.31D-26
23	O3 + HO2 >>> HO + 2*O2	1.18D-14	1.12D-49
24	H + HO + M >>> H2O + M	3.37D-15	8.10D-28
25	H + HO2 >>> 2*HO	1.08D-10	5.87D-24
26	H + HO2 >>> H2 + O2	2.55D-11	8.03D-29
27	H + H2O >>> H2 + HO	6.56D-17	8.90D-13
28	H + H2O2 >>> H2 + HO2	3.06D-13	1.77D-18
29	H + H2O2 >>> HO + H2O	3.98D-13	1.02D-35
30	2*HO + M >>> H2O2 + M	2.76D-15	2.53D-05
31	HO + HO2 >>> H2O + O2	4.06D-11	7.73D-33
32	2*HO2 >>> H2O2 + O2	4.32D-12	3.02D-24
33	HO2 + H2O >>> H2O2 + HO	2.72D-21	3.07D-12
34	NO + H + M >>> HNO + M	7.04D-16	5.32D-07
35	NO + HO >>> NO2 + H	2.23D-21	2.02D-10
36	NO + HO + M >>> HNO2 + M	1.15D-14	1.43D-03
37	NO + HO2 >>> NO2 + HO	3.60D-12	2.68D-14
38	H + H + M >>> H2 + M	6.11D-17	5.12D-26
39	HNO4 + M >>> HO2 + NO2 + M	1.76D 05	1.65D-15
40	CLNO3 + M >>> CLO + NO2 + M	9.08D 04	6.53D-16

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	5.500D 07	2.200D 09	2.000D 06	5.500D 08	1.300D 12	3.800D 16	5.000D 07	5.000D 06	5.300D 11
0.20	1.277D-03	2.100D 09	5.917D 07	9.727D 08	1.100D 12	3.800D 16	4.990D 07	1.217D 08	5.300D 11
0.40	8.250D-04	1.325D 09	6.059D 07	1.747D 09	9.259D 11	3.800D 16	4.981D 07	1.985D 08	5.300D 11
0.60	4.574D-04	7.283D 08	6.111D 07	2.343D 09	7.815D 11	3.800D 16	4.971D 07	2.149D 08	5.300D 11
0.80	2.441D-04	3.891D 08	6.105D 07	2.682D 09	6.641D 11	3.800D 16	4.962D 07	2.244D 08	5.300D 11
1.00	1.379D-04	2.211D 08	6.068D 07	2.851D 09	5.697D 11	3.800D 16	4.952D 07	2.348D 08	5.300D 11
1.20	8.761D-05	1.416D 08	6.017D 07	2.931D 09	4.943D 11	3.800D 16	4.942D 07	2.461D 08	5.300D 11
1.40	6.320D-05	1.032D 08	5.961D 07	2.970D 09	4.342D 11	3.800D 16	4.933D 07	2.580D 08	5.300D 11
1.60	5.041D-05	8.311D 07	5.901D 07	2.991D 09	3.861D 11	3.800D 16	4.923D 07	2.703D 08	5.299D 11
1.80	4.298D-05	7.161D 07	5.840D 07	3.003D 09	3.474D 11	3.800D 16	4.914D 07	2.828D 08	5.299D 11
2.00	3.822D-05	6.435D 07	5.779D 07	3.011D 09	3.161D 11	3.800D 16	4.904D 07	2.953D 08	5.299D 11
2.20	3.492D-05	5.942D 07	5.717D 07	3.016D 09	2.905D 11	3.800D 16	4.895D 07	3.077D 08	5.299D 11
2.40	3.250D-05	5.591D 07	5.656D 07	3.021D 09	2.694D 11	3.800D 16	4.885D 07	3.200D 08	5.299D 11
2.60	3.067D-05	5.334D 07	5.595D 07	3.024D 09	2.518D 11	3.800D 16	4.876D 07	3.321D 08	5.299D 11
2.80	2.925D-05	5.142D 07	5.534D 07	3.027D 09	2.369D 11	3.800D 16	4.866D 07	3.439D 08	5.299D 11
3.00	2.812D-05	4.997D 07	5.474D 07	3.029D 09	2.242D 11	3.800D 16	4.857D 07	3.554D 08	5.299D 11
3.20	2.721D-05	4.889D 07	5.414D 07	3.030D 09	2.132D 11	3.800D 16	4.847D 07	3.666D 08	5.299D 11
3.40	2.646D-05	4.808D 07	5.355D 07	3.032D 09	2.035D 11	3.800D 16	4.838D 07	3.775D 08	5.299D 11
3.60	2.585D-05	4.748D 07	5.296D 07	3.033D 09	1.950D 11	3.800D 16	4.828D 07	3.880D 08	5.299D 11
3.80	2.533D-05	4.705D 07	5.238D 07	3.034D 09	1.874D 11	3.800D 16	4.819D 07	3.982D 08	5.299D 11
4.00	2.488D-05	4.674D 07	5.180D 07	3.035D 09	1.806D 11	3.800D 16	4.810D 07	4.081D 08	5.299D 11
4.20	2.450D-05	4.653D 07	5.123D 07	3.036D 09	1.743D 11	3.800D 16	4.800D 07	4.176D 08	5.298D 11
4.40	2.416D-05	4.640D 07	5.066D 07	3.037D 09	1.686D 11	3.800D 16	4.791D 07	4.269D 08	5.298D 11
4.60	2.386D-05	4.633D 07	5.010D 07	3.038D 09	1.633D 11	3.800D 16	4.782D 07	4.358D 08	5.298D 11
4.80	2.358D-05	4.630D 07	4.955D 07	3.038D 09	1.584D 11	3.800D 16	4.772D 07	4.444D 08	5.298D 11
5.00	2.332D-05	4.631D 07	4.900D 07	3.039D 09	1.538D 11	3.800D 16	4.763D 07	4.528D 08	5.298D 11
5.20	2.308D-05	4.635D 07	4.846D 07	3.040D 09	1.495D 11	3.800D 16	4.754D 07	4.608D 08	5.298D 11
5.40	2.286D-05	4.641D 07	4.792D 07	3.040D 09	1.455D 11	3.800D 16	4.745D 07	4.686D 08	5.298D 11
5.60	2.264D-05	4.648D 07	4.739D 07	3.041D 09	1.417D 11	3.800D 16	4.735D 07	4.762D 08	5.298D 11
5.80	2.243D-05	4.657D 07	4.686D 07	3.041D 09	1.381D 11	3.800D 16	4.726D 07	4.834D 08	5.298D 11
6.00	2.223D-05	4.667D 07	4.634D 07	3.042D 09	1.346D 11	3.800D 16	4.717D 07	4.905D 08	5.298D 11
6.20	2.203D-05	4.677D 07	4.582D 07	3.042D 09	1.314D 11	3.800D 16	4.708D 07	4.973D 08	5.298D 11
6.40	2.183D-05	4.687D 07	4.531D 07	3.043D 09	1.283D 11	3.800D 16	4.699D 07	5.039D 08	5.298D 11
6.60	2.164D-05	4.698D 07	4.481D 07	3.043D 09	1.253D 11	3.800D 16	4.689D 07	5.102D 08	5.298D 11
6.80	2.145D-05	4.709D 07	4.431D 07	3.044D 09	1.225D 11	3.800D 16	4.680D 07	5.164D 08	5.298D 11
7.00	2.126D-05	4.720D 07	4.382D 07	3.044D 09	1.198D 11	3.800D 16	4.671D 07	5.224D 08	5.298D 11
7.20	2.107D-05	4.731D 07	4.333D 07	3.045D 09	1.172D 11	3.800D 16	4.662D 07	5.281D 08	5.298D 11
7.40	2.088D-05	4.742D 07	4.284D 07	3.045D 09	1.147D 11	3.800D 16	4.653D 07	5.337D 08	5.298D 11
7.60	2.069D-05	4.752D 07	4.237D 07	3.046D 09	1.123D 11	3.800D 16	4.644D 07	5.391D 08	5.298D 11
7.80	2.051D-05	4.763D 07	4.189D 07	3.046D 09	1.100D 11	3.800D 16	4.635D 07	5.444D 08	5.298D 11
8.00	2.032D-05	4.774D 07	4.143D 07	3.046D 09	1.078D 11	3.800D 16	4.626D 07	5.494D 08	5.298D 11
8.20	2.014D-05	4.784D 07	4.096D 07	3.047D 09	1.056D 11	3.800D 16	4.617D 07	5.543D 08	5.298D 11
8.40	1.996D-05	4.794D 07	4.050D 07	3.047D 09	1.036D 11	3.800D 16	4.608D 07	5.591D 08	5.298D 11
8.60	1.978D-05	4.804D 07	4.005D 07	3.048D 09	1.016D 11	3.800D 16	4.599D 07	5.637D 08	5.298D 11
8.80	1.959D-05	4.814D 07	3.960D 07	3.048D 09	9.971D 10	3.800D 16	4.590D 07	5.682D 08	5.298D 11
9.00	1.941D-05	4.823D 07	3.916D 07	3.049D 09	9.786D 10	3.800D 16	4.581D 07	5.725D 08	5.298D 11
9.20	1.923D-05	4.832D 07	3.872D 07	3.049D 09	9.608D 10	3.800D 16	4.572D 07	5.767D 08	5.298D 11
9.40	1.905D-05	4.842D 07	3.829D 07	3.050D 09	9.436D 10	3.800D 16	4.563D 07	5.808D 08	5.298D 11
9.60	1.887D-05	4.851D 07	3.786D 07	3.050D 09	9.269D 10	3.800D 16	4.555D 07	5.847D 08	5.298D 11
9.80	1.870D-05	4.859D 07	3.744D 07	3.050D 09	9.108D 10	3.800D 16	4.546D 07	5.885D 08	5.297D 11
10.00	1.852D-05	4.868D 07	3.702D 07	3.051D 09	8.952D 10	3.800D 16	4.537D 07	5.922D 08	5.297D 11

TIME(S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000D 06	1.0000D 06	1.0000D 06	1.7000D 07	2.8000D 08	1.0000D 06	7.0000D 05	2.3000D 08	4.0000D 07
0.20	1.6950D 11	5.1420D 06	1.0010D 06	1.3000D 08	2.8010D 08	1.0000D 06	6.9990D 05	2.5530D-03	1.3590D-03
0.40	2.7690D 11	1.5140D 07	1.0060D 06	5.1580D 07	2.8000D 08	1.0000D 06	7.0020D 05	5.6360D-04	8.5730D-04
0.60	3.4440D 11	2.1560D 07	1.0100D 06	4.4840D 07	2.8000D 08	1.0000D 06	7.0100D 05	3.0530D-04	4.7130D-04
0.80	3.8560D 11	2.6320D 07	1.0170D 06	4.6690D 07	2.8000D 08	1.0000D 06	7.0210D 05	1.6980D-04	2.5180D-04
1.00	4.0930D 11	3.0260D 07	1.0240D 06	4.9710D 07	2.7990D 08	1.0000D 06	7.0340D 05	1.0280D-04	1.4310D-04
1.20	4.2100D 11	3.3570D 07	1.0330D 06	5.3070D 07	2.7990D 08	1.0000D 06	7.0480D 05	7.0270D-05	9.1660D-05
1.40	4.2450D 11	3.6320D 07	1.0440D 06	5.6580D 07	2.7980D 08	1.0000D 06	7.0630D 05	5.4550D-05	6.6750D-05
1.60	4.2250D 11	3.8590D 07	1.0560D 06	6.0140D 07	2.7980D 08	1.0000D 06	7.0790D 05	4.6730D-05	5.3780D-05
1.80	4.1660D 11	4.0440D 07	1.0690D 06	6.3710D 07	2.7980D 08	1.0000D 06	7.0960D 05	4.2650D-05	4.6340D-05
2.00	4.0930D 11	4.1910D 07	1.0840D 06	6.7240D 07	2.7970D 08	1.0000D 06	7.1140D 05	4.0450D-05	4.1640D-05
2.20	3.9830D 11	4.3060D 07	1.1000D 06	7.0710D 07	2.7970D 08	1.0000D 06	7.1330D 05	3.9280D-05	3.8450D-05
2.40	3.8740D 11	4.3930D 07	1.1170D 06	7.4110D 07	2.7960D 08	1.0000D 06	7.1530D 05	3.8730D-05	3.6180D-05
2.60	3.7600D 11	4.4570D 07	1.1350D 06	7.7420D 07	2.7960D 08	1.0000D 06	7.1730D 05	3.8600D-05	3.4510D-05
2.80	3.6440D 11	4.5010D 07	1.1540D 06	8.0630D 07	2.7950D 08	1.0000D 06	7.1950D 05	3.8750D-05	3.3270D-05
3.00	3.5290D 11	4.5290D 07	1.1740D 06	8.3750D 07	2.7950D 08	1.0000D 06	7.2170D 05	3.9120D-05	3.2340D-05
3.20	3.4150D 11	4.5430D 07	1.1950D 06	8.6780D 07	2.7940D 08	1.0000D 06	7.2400D 05	3.9660D-05	3.1640D-05
3.40	3.3050D 11	4.5460D 07	1.2160D 06	8.9710D 07	2.7940D 08	1.0000D 06	7.2640D 05	4.0320D-05	3.1110D-05
3.60	3.1990D 11	4.5390D 07	1.2380D 06	9.2540D 07	2.7930D 08	1.0000D 06	7.2890D 05	4.1080D-05	3.0730D-05
3.80	3.0970D 11	4.5240D 07	1.2610D 06	9.5280D 07	2.7930D 08	1.0000D 06	7.3140D 05	4.1910D-05	3.0440D-05
4.00	2.9990D 11	4.5030D 07	1.2840D 06	9.7940D 07	2.7920D 08	1.0000D 06	7.3400D 05	4.2790D-05	3.0250D-05
4.20	2.9060D 11	4.4770D 07	1.3080D 06	1.0050D 08	2.7910D 08	1.0000D 06	7.3670D 05	4.3720D-05	3.0110D-05
4.40	2.8170D 11	4.4470D 07	1.3320D 06	1.0300D 08	2.7910D 08	1.0000D 06	7.3950D 05	4.4670D-05	3.0020D-05
4.60	2.7330D 11	4.4140D 07	1.3560D 06	1.0540D 08	2.7900D 08	1.0000D 06	7.4230D 05	4.5640D-05	2.9980D-05
4.80	2.6520D 11	4.3780D 07	1.3810D 06	1.0770D 08	2.7900D 08	1.0000D 06	7.4510D 05	4.6620D-05	2.9960D-05
5.00	2.5760D 11	4.3400D 07	1.4060D 06	1.0990D 08	2.7890D 08	1.0000D 06	7.4810D 05	4.7600D-05	2.9970D-05
5.20	2.5030D 11	4.3000D 07	1.4320D 06	1.1210D 08	2.7880D 08	1.0000D 06	7.5110D 05	4.8580D-05	2.9990D-05
5.40	2.4330D 11	4.2590D 07	1.4570D 06	1.1420D 08	2.7880D 08	1.0000D 06	7.5410D 05	4.9550D-05	3.0030D-05
5.60	2.3680D 11	4.2170D 07	1.4830D 06	1.1630D 08	2.7870D 08	1.0000D 06	7.5720D 05	5.0510D-05	3.0080D-05
5.80	2.3050D 11	4.1740D 07	1.5090D 06	1.1820D 08	2.7870D 08	1.0000D 06	7.6030D 05	5.1460D-05	3.0130D-05
6.00	2.2450D 11	4.1310D 07	1.5350D 06	1.2010D 08	2.7860D 08	1.0000D 06	7.6350D 05	5.2400D-05	3.0200D-05
6.20	2.1880D 11	4.0880D 07	1.5610D 06	1.2200D 08	2.7850D 08	1.0000D 06	7.6680D 05	5.3320D-05	3.0260D-05
6.40	2.1340D 11	4.0450D 07	1.5880D 06	1.2380D 08	2.7850D 08	1.0010D 06	7.7010D 05	5.4220D-05	3.0330D-05
6.60	2.0820D 11	4.0010D 07	1.6140D 06	1.2550D 08	2.7840D 08	1.0010D 06	7.7340D 05	5.5110D-05	3.0400D-05
6.80	2.0320D 11	3.9580D 07	1.6400D 06	1.2720D 08	2.7830D 08	1.0010D 06	7.7680D 05	5.5970D-05	3.0470D-05
7.00	1.9850D 11	3.9140D 07	1.6670D 06	1.2880D 08	2.7830D 08	1.0010D 06	7.8020D 05	5.6820D-05	3.0540D-05
7.20	1.9390D 11	3.8710D 07	1.6930D 06	1.3030D 08	2.7820D 08	1.0010D 06	7.8370D 05	5.7640D-05	3.0610D-05
7.40	1.8960D 11	3.8290D 07	1.7200D 06	1.3190D 08	2.7810D 08	1.0010D 06	7.8720D 05	5.8450D-05	3.0680D-05
7.60	1.8540D 11	3.7860D 07	1.7460D 06	1.3330D 08	2.7810D 08	1.0010D 06	7.9070D 05	5.9240D-05	3.0750D-05
7.80	1.8140D 11	3.7440D 07	1.7730D 06	1.3480D 08	2.7800D 08	1.0010D 06	7.9430D 05	6.0010D-05	3.0820D-05
8.00	1.7750D 11	3.7030D 07	1.7990D 06	1.3620D 08	2.7790D 08	1.0010D 06	7.9790D 05	6.0760D-05	3.0890D-05
8.20	1.7380D 11	3.6610D 07	1.8250D 06	1.3750D 08	2.7790D 08	1.0010D 06	8.0150D 05	6.1490D-05	3.0960D-05
8.40	1.7030D 11	3.6200D 07	1.8520D 06	1.3880D 08	2.7780D 08	1.0010D 06	8.0520D 05	6.2210D-05	3.1020D-05
8.60	1.6690D 11	3.5800D 07	1.8780D 06	1.4010D 08	2.7780D 08	1.0010D 06	8.0890D 05	6.2900D-05	3.1080D-05
8.80	1.6360D 11	3.5400D 07	1.9040D 06	1.4130D 08	2.7770D 08	1.0010D 06	8.1270D 05	6.3580D-05	3.1150D-05
9.00	1.6040D 11	3.5010D 07	1.9300D 06	1.4250D 08	2.7760D 08	1.0010D 06	8.1640D 05	6.4240D-05	3.1210D-05
9.20	1.5740D 11	3.4620D 07	1.9560D 06	1.4360D 08	2.7760D 08	1.0010D 06	8.2020D 05	6.4890D-05	3.1270D-05
9.40	1.5440D 11	3.4230D 07	1.9820D 06	1.4480D 08	2.7750D 08	1.0010D 06	8.2410D 05	6.5520D-05	3.1330D-05
9.60	1.5160D 11	3.3860D 07	2.0080D 06	1.4580D 08	2.7740D 08	1.0010D 06	8.2790D 05	6.6130D-05	3.1390D-05
9.80	1.4880D 11	3.3480D 07	2.0340D 06	1.4690D 08	2.7740D 08	1.0010D 06	8.3180D 05	6.6730D-05	3.1440D-05
10.00	1.4610D 11	3.3110D 07	2.0590D 06	1.4790D 08	2.7730D 08	1.0010D 06	8.3570D 05	6.7310D-05	3.1500D-05

T=800 K, H=35 km

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	6.42D 05	8.97D-16
2	2*NO3 >>> 2*NO2 + O2	3.98D-14	5.95D-48
3	NO2 + NO3 >>> NO2 + NO + O2	6.59D-14	3.13D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.74D-18
5	NO + O3 >>> NO2 + O2	3.43D-13	4.42D-26
6	NO2 + O3 >>> NO3 + O2	5.61D-15	9.78D-21
7	HNO3 + M >>> HO + NO2 + M	4.60D-01	1.02D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	2.43D-18
9	O + O + M >>> O2 + M	1.71D-17	1.10D-17
10	O + O2 + M >>> O3 + M	1.07D-17	5.47D 00
11	O + O3 >>> 2*O2	1.07D-12	6.11D-39
12	O + NO + M >>> NO2 + M	1.72D-15	1.64D-09
13	O + NO2 >>> NO + O2	1.17D-11	5.55D-25
14	O + NO2 + M >>> NO3 + M	5.35D-15	4.28D-25
15	HO + HO >>> H2O + O	5.00D-12	1.06D-15
16	O2 + 2*NO >>> 2*NO2	6.40D-39	8.78D-20
17	NO2 + H-NU >>> NO + O	0.0	0.0
18	O + HO >>> H + O2	4.20D-11	9.55D-15
19	O + HO2 >>> HO + O2	4.28D-11	3.43D-26
20	O2 + H + M >>> HO2 + M	5.33D-16	7.95D-05
21	O3 + H >>> HO + O2	5.25D-11	6.31D-34
22	O3 + HO >>> HO2 + O2	4.30D-13	3.24D-24
23	O3 + HO2 >>> HO + 2*O2	1.48D-14	2.35D-48
24	H + HO + M >>> H2O + M	2.08D-15	2.06D-23
25	H + HO2 >>> 2*HO	1.28D-10	2.16D-22
26	H + HO2 >>> H2 + O2	2.71D-11	1.45D-26
27	H + H2O >>> H2 + HO	4.09D-16	1.41D-12
28	H + H2O2 >>> H2 + HO2	3.93D-13	9.47D-18
29	+ H2O2 >>> HO + H2O	5.11D-13	6.02D-39
30	2*HO + M >>> H2O2 + M	2.06D-15	1.70D-03
31	HO + HO2 >>> H2O + O2	4.44D-11	5.70D-30
32	2*HO2 >>> H2O2 + O2	9.10D-12	1.53D-22
33	HO2 + H2O >>> H2O2 + HO	5.19D-20	3.46D-12
34	NO + H + M >>> HNO + M	5.84D-16	3.47D-05
35	NO + HO >>> NO2 + H	3.30D-20	2.30D-10
36	NO + HO + M >>> HNO2 + M	8.27D-15	7.88D-02
37	NO + HO2 >>> NO2 + HO	4.46D-12	7.66D-14
38	H + H + M >>> H2 + M	5.35D-17	5.64D-22
39	HNO4 + M >>> HO2 + NO2 + M	9.25D 05	1.21D-15
40	CLNO3 + M >>> CLO + NO2 + M	5.87D 05	3.77D-16

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	5.500D 07	2.200D 09	2.000D 06	5.500D 08	1.300D 12	3.800D 16	5.000D 07	5.000D 06	5.300D 11
0.20	7.377D-05	8.922D 08	5.921D 07	2.185D 09	4.190D 11	3.800D 16	4.561D 07	3.173D 08	5.299D 11
0.40	1.167D-05	1.414D 08	5.911D 07	2.740D 09	1.566D 11	3.800D 16	4.161D 07	4.859D 08	5.299D 11
0.60	2.205D-06	2.694D 07	5.851D 07	3.059D 09	8.560D 10	3.800D 16	3.795D 07	6.686D 08	5.297D 11
0.80	9.219D-07	1.141D 07	5.784D 07	3.078D 09	6.611D 10	3.800D 16	3.462D 07	8.530D 08	5.296D 11
1.00	7.138D-07	8.949D 06	5.718D 07	3.084D 09	6.011D 10	3.800D 16	3.158D 07	1.034D 09	5.295D 11
1.20	6.654D-07	8.431D 06	5.652D 07	3.088D 09	5.765D 10	3.800D 16	2.881D 07	1.211D 09	5.294D 11
1.40	6.464D-07	8.286D 06	5.586D 07	3.092D 09	5.613D 10	3.800D 16	2.628D 07	1.383D 09	5.293D 11
1.60	6.342D-07	8.225D 06	5.521D 07	3.095D 09	5.489D 10	3.800D 16	2.397D 07	1.551D 09	5.293D 11
1.80	6.239D-07	8.188D 06	5.457D 07	3.097D 09	5.375D 10	3.800D 16	2.186D 07	1.713D 09	5.292D 11
2.00	6.145D-07	8.159D 06	5.394D 07	3.100D 09	5.266D 10	3.800D 16	1.994D 07	1.870D 09	5.291D 11
2.20	6.056D-07	8.136D 06	5.331D 07	3.102D 09	5.160D 10	3.800D 16	1.819D 07	2.022D 09	5.290D 11
2.40	5.971D-07	8.116D 06	5.269D 07	3.105D 09	5.058D 10	3.800D 16	1.659D 07	2.170D 09	5.289D 11
2.60	5.890D-07	8.100D 06	5.207D 07	3.107D 09	4.958D 10	3.800D 16	1.514D 07	2.312D 09	5.288D 11
2.80	5.812D-07	8.087D 06	5.146D 07	3.109D 09	4.862D 10	3.800D 16	1.381D 07	2.450D 09	5.288D 11
3.00	5.735D-07	8.076D 06	5.086D 07	3.111D 09	4.768D 10	3.800D 16	1.259D 07	2.583D 09	5.287D 11
3.20	5.664D-07	8.068D 06	5.027D 07	3.112D 09	4.677D 10	3.800D 16	1.149D 07	2.711D 09	5.286D 11
3.40	5.594D-07	8.063D 06	4.968D 07	3.114D 09	4.589D 10	3.800D 16	1.048D 07	2.835D 09	5.286D 11
3.60	5.526D-07	8.060D 06	4.910D 07	3.115D 09	4.503D 10	3.800D 16	9.557D 06	2.954D 09	5.285D 11
3.80	5.461D-07	8.059D 06	4.852D 07	3.117D 09	4.420D 10	3.800D 16	8.718D 06	3.068D 09	5.284D 11
4.00	5.398D-07	8.060D 06	4.796D 07	3.118D 09	4.338D 10	3.800D 16	7.952D 06	3.178D 09	5.284D 11
4.20	5.337D-07	8.063D 06	4.739D 07	3.119D 09	4.259D 10	3.800D 16	7.253D 06	3.283D 09	5.283D 11
4.40	5.277D-07	8.068D 06	4.684D 07	3.120D 09	4.182D 10	3.800D 16	6.616D 06	3.384D 09	5.283D 11
4.60	5.219D-07	8.074D 06	4.629D 07	3.122D 09	4.108D 10	3.800D 16	6.035D 06	3.481D 09	5.282D 11
4.80	5.163D-07	8.082D 06	4.574D 07	3.123D 09	4.035D 10	3.800D 16	5.505D 06	3.574D 09	5.282D 11
5.00	5.108D-07	8.091D 06	4.521D 07	3.124D 09	3.964D 10	3.800D 16	5.021D 06	3.663D 09	5.281D 11
5.20	5.054D-07	8.102D 06	4.468D 07	3.125D 09	3.895D 10	3.800D 16	4.580D 06	3.747D 09	5.281D 11
5.40	5.002D-07	8.113D 06	4.415D 07	3.126D 09	3.828D 10	3.800D 16	4.178D 06	3.828D 09	5.280D 11
5.60	4.951D-07	8.126D 06	4.363D 07	3.126D 09	3.762D 10	3.800D 16	3.811D 06	3.906D 09	5.280D 11
5.80	4.901D-07	8.140D 06	4.312D 07	3.127D 09	3.699D 10	3.800D 16	3.476D 06	3.979D 09	5.280D 11
6.00	4.852D-07	8.154D 06	4.261D 07	3.128D 09	3.637D 10	3.800D 16	3.171D 06	4.049D 09	5.279D 11
6.20	4.804D-07	8.169D 06	4.211D 07	3.129D 09	3.576D 10	3.800D 16	2.892D 06	4.115D 09	5.279D 11
6.40	4.756D-07	8.185D 06	4.161D 07	3..29D 09	3.517D 10	3.800D 16	2.638D 06	4.179D 09	5.278D 11
6.60	4.710D-07	8.202D 06	4.112D 07	3.130D 09	3.460D 10	3.800D 16	2.406D 06	4.238D 09	5.278D 11
6.80	4.664D-07	8.219D 06	4.064D 07	3.131D 09	3.403D 10	3.800D 16	2.195D 06	4.295D 09	5.278D 11
7.00	4.619D-07	8.237D 06	4.016D 07	3.132D 09	3.349D 10	3.800D 16	2.002D 06	4.349D 09	5.278D 11
7.20	4.575D-07	8.255D 06	3.969D 07	3.132D 09	3.295D 10	3.800D 16	1.826D 06	4.399D 09	5.277D 11
7.40	4.531D-07	8.273D 06	3.922D 07	3.133D 09	3.243D 10	3.800D 16	1.666D 06	4.447D 09	5.277D 11
7.60	4.488D-07	8.292D 06	3.876D 07	3.133D 09	3.193D 10	3.800D 16	1.520D 06	4.492D 09	5.277D 11
7.80	4.445D-07	8.312D 06	3.830D 07	3.134D 09	3.143D 10	3.800D 16	1.386D 06	4.534D 09	5.277D 11
8.00	4.403D-07	8.331D 06	3.785D 07	3.134D 09	3.095D 10	3.800D 16	1.264D 06	4.574D 09	5.277D 11
8.20	4.361D-07	8.351D 06	3.740D 07	3.135D 09	3.047D 10	3.800D 16	1.153D 06	4.611D 09	5.276D 11
8.40	4.320D-07	8.371D 06	3.696D 07	3.135D 09	3.001D 10	3.800D 16	1.052D 06	4.646D 09	5.276D 11
8.60	4.279D-07	8.391D 06	3.652D 07	3.136D 09	2.956D 10	3.800D 16	9.597D 05	4.679D 09	5.276D 11
8.80	4.239D-07	8.411D 06	3.609D 07	3.136D 09	2.912D 10	3.800D 16	8.754D 05	4.709D 09	5.276D 11
9.00	4.199D-07	8.431D 06	3.566D 07	3.137D 09	2.870D 10	3.800D 16	7.986D 05	4.737D 09	5.276D 11
9.20	4.159D-07	8.451D 06	3.524D 07	3.137D 09	2.828D 10	3.800D 16	7.285D 05	4.763D 09	5.276D 11
9.40	4.120D-07	8.472D 06	3.483D 07	3.138D 09	2.787D 10	3.800D 16	6.646D 05	4.787D 09	5.276D 11
9.60	4.081D-07	8.492D 06	3.442D 07	3.138D 09	2.747D 10	3.800D 16	6.062D 05	4.809D 09	5.275D 11
9.80	4.043D-07	8.512D 06	3.401D 07	3.139D 09	2.707D 10	3.800D 16	5.530D 05	4.830D 09	5.275D 11
10.00	4.004D-07	8.533D 06	3.361D 07	3.139D 09	2.669D 10	3.800D 16	5.045D 05	4.848D 09	5.275D 11

TIME (S)	O	H	H2	HO2	H2O2	HNO	HNO2	HNO4	CLNO3
0.0	1.0000 06	1.0000 06	1.0000 06	1.7000 07	2.8000 08	1.0000 06	7.0000 05	2.3000 08	4.0000 07
0.20	7.4750 11	2.4280 07	1.0030 06	2.0120 07	2.7990 08	1.0000 06	6.8950 05	2.3500-05	5.1590-05
0.40	9.1470 11	4.7430 07	1.0100 06	2.4210 07	2.7970 08	1.0000 06	6.8050 05	4.4800-06	8.1760-06
0.60	9.3950 11	6.7830 07	1.0220 06	3.3560 07	2.7950 08	1.0000 06	6.7270 05	1.1850-06	1.5610-06
0.80	9.2840 11	8.5830 07	1.0430 06	4.3110 07	2.7930 08	1.0000 06	6.6600 05	6.4390-07	6.6000-07
1.00	9.0870 11	1.0200 08	1.0740 06	5.2530 07	2.7900 08	1.0000 06	6.6040 05	6.1460-07	5.1690-07
1.20	8.8740 11	1.1670 08	1.1140 06	6.1740 07	2.7870 08	1.0000 06	6.5580 05	6.8120-07	4.8750-07
1.40	8.6630 11	1.3020 08	1.1660 06	7.0690 07	2.7830 08	1.0000 06	6.5210 05	7.6670-07	4.7910-07
1.60	8.4570 11	1.4260 08	1.2300 06	7.9400 07	2.7800 08	1.0000 06	6.4930 05	8.5470-07	4.7560-07
1.80	8.2590 11	1.5380 08	1.3070 06	8.7840 07	2.7760 08	1.0000 06	6.4750 05	9.4120-07	4.7340-07
2.00	8.0680 11	1.6410 08	1.3960 06	9.6020 07	2.7710 08	1.0000 06	6.4650 05	1.0250-06	4.7180-07
2.20	7.8830 11	1.7350 08	1.4980 06	1.0390 08	2.7670 08	1.0000 06	6.4630 05	1.1070-06	4.7040-07
2.40	7.7050 11	1.8190 08	1.6120 06	1.1160 08	2.7620 08	1.0000 06	6.4680 05	1.1860-06	4.6930-07
2.60	7.5330 11	1.8960 08	1.7400 06	1.1900 08	2.7570 08	1.0000 06	6.4810 05	1.2620-06	4.6840-07
2.80	7.3670 11	1.9650 08	1.8790 06	1.2620 08	2.7520 08	1.0010 06	6.5020 05	1.3350-06	4.6760-07
3.00	7.2060 11	2.0270 08	2.0310 06	1.3310 08	2.7460 08	1.0010 06	6.5280 05	1.4070-06	4.6700-07
3.20	7.0510 11	2.0820 08	2.1950 06	1.3970 08	2.7400 08	1.0010 06	6.5610 05	1.4760-06	4.6660-07
3.40	6.9010 11	2.1310 08	2.3700 06	1.4620 08	2.7350 08	1.0010 06	6.6010 05	1.5420-06	4.6620-07
3.60	6.7560 11	2.1740 08	2.5560 06	1.5230 08	2.7290 08	1.0010 06	6.6450 05	1.6070-06	4.6610-07
3.80	6.6160 11	2.2110 08	2.7530 06	1.5830 08	2.7220 08	1.0010 06	6.6950 05	1.6690-06	4.6600-07
4.00	6.4800 11	2.2440 08	2.9600 06	1.6400 08	2.7160 08	1.0010 06	6.7500 05	1.7300-06	4.6610-07
4.20	6.3480 11	2.2710 08	3.1760 06	1.6940 08	2.7090 08	1.0010 06	6.8100 05	1.7880-06	4.6630-07
4.40	6.2210 11	2.2950 08	3.4000 06	1.7470 08	2.7030 08	1.0010 06	6.8740 05	1.8440-06	4.6650-07
4.60	6.0970 11	2.3140 08	3.6330 06	1.7970 08	2.6960 08	1.0010 06	6.9430 05	1.8990-06	4.6690-07
4.80	5.9770 11	2.3290 08	3.8740 06	1.8450 08	2.6890 08	1.0010 06	7.0150 05	1.9510-06	4.6730-07
5.00	5.8610 11	2.3410 08	4.1210 06	1.8910 08	2.6820 08	1.0010 06	7.0910 05	2.0020-06	4.6790-07
5.20	5.7480 11	2.3490 08	4.3750 06	1.9350 08	2.6750 08	1.0010 06	7.1700 05	2.0510-06	4.6850-07
5.40	5.6390 11	2.3540 08	4.6350 06	1.9760 08	2.6670 08	1.0010 06	7.2520 05	2.0990-06	4.6910-07
5.60	5.5330 11	2.3570 08	4.9000 06	2.0160 08	2.6600 08	1.0020 06	7.3370 05	2.1440-06	4.6990-07
5.80	5.4300 11	2.3570 08	5.1690 06	2.0540 08	2.6530 08	1.0020 06	7.4240 05	2.1880-06	4.7070-07
6.00	5.3300 11	2.3540 08	5.4430 06	2.0900 08	2.6450 08	1.0020 06	7.5140 05	2.2310-06	4.7150-07
6.20	5.2330 11	2.3490 08	5.7210 06	2.1250 08	2.6370 08	1.0020 06	7.6070 05	2.2720-06	4.7240-07
6.40	5.1380 11	2.3430 08	6.0010 06	2.1570 08	2.6300 08	1.0020 06	7.7010 05	2.3110-06	4.7330-07
6.60	5.0460 11	2.3340 08	6.2840 06	2.1880 08	2.6220 08	1.0020 06	7.7960 05	2.3490-06	4.7430-07
6.80	4.9570 11	2.3230 08	6.5700 06	2.2170 08	2.6140 08	1.0020 06	7.8940 05	2.3850-06	4.7520-07
7.00	4.8700 11	2.3120 08	6.8570 06	2.2450 08	2.6060 08	1.0020 06	7.9920 05	2.4200-06	4.7630-07
7.20	4.7860 11	2.2980 08	7.1450 06	2.2710 08	2.5990 08	1.0020 06	8.0920 05	2.4530-06	4.7730-07
7.40	4.7040 11	2.2830 08	7.4340 06	2.2950 08	2.5910 08	1.0020 06	8.1930 05	2.4850-06	4.7840-07
7.60	4.6240 11	2.2680 08	7.7240 06	2.3180 08	2.5830 08	1.0020 06	8.2950 05	2.5160-06	4.7950-07
7.80	4.5460 11	2.2510 08	8.0130 06	2.3400 08	2.5750 08	1.0020 06	8.3970 05	2.5450-06	4.8060-07
8.00	4.4710 11	2.2330 08	8.3030 06	2.3600 08	2.5670 08	1.0020 06	8.5000 05	2.5740-06	4.8170-07
8.20	4.3970 11	2.2140 08	8.5920 06	2.3790 08	2.5590 08	1.0030 06	8.6030 05	2.6000-06	4.8290-07
8.40	4.3250 11	2.1940 08	8.8800 06	2.3970 08	2.5510 08	1.0030 06	8.7070 05	2.6260-06	4.8400-07
8.60	4.2550 11	2.1740 08	9.1670 06	2.4140 08	2.5430 08	1.0030 06	8.8110 05	2.6510-06	4.8520-07
8.80	4.1870 11	2.1530 08	9.4520 06	2.4290 08	2.5350 08	1.0030 06	8.9140 05	2.6740-06	4.8630-07
9.00	4.1210 11	2.1320 08	9.7360 06	2.4430 08	2.5260 08	1.0030 06	9.0180 05	2.6960-06	4.8750-07
9.20	4.0560 11	2.1100 08	1.0020 07	2.4570 08	2.5180 08	1.0030 06	9.1220 05	2.7170-06	4.8870-07
9.40	3.9930 11	2.0880 08	1.0300 07	2.4690 08	2.5100 08	1.0030 06	9.2250 05	2.7370-06	4.8990-07
9.60	3.9320 11	2.0660 08	1.0580 07	2.4800 08	2.5020 08	1.0030 06	9.3280 05	2.7560-06	4.9100-07
9.80	3.8720 11	2.0430 08	1.0850 07	2.4900 08	2.4940 08	1.0030 06	9.4300 05	2.7740-06	4.9220-07
10.00	3.8130 11	2.0200 08	1.1120 07	2.5000 08	2.4860 08	1.0030 06	9.5320 05	2.7910-06	4.9340-07

25 km HNO_3, N_2O_5, O

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N205 + M >>> NO2 +NO3 + M	4.05D-06	1.27D-13
2	2*NO3 >>> 2*NO2 + O2	4.71D-17	7.46D-62
3	NO2 + NO3 >>> NO2 + NO + O2	4.21D-15	1.19D-34
4	NO3 + NO >>> 2*NO2	1.90D-11	3.29D-32
5	NO + O3 >>> NO2 + O2	6.36D-15	1.08D-56
6	NO2 + O3 >>> NO3 + O2	6.65D-18	8.33D-39
7	HNO3 + M >>> HO + NO2 + M	5.36D-28	2.46D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	3.76D-30
9	O + O + M >>> O2 + M	2.69D-15	1.44D-57
10	O + O2 + M >>> O3 + M	5.76D-16	1.62D-12
11	O + O3 >>> 2*O2	1.92D-15	0.0
12	O + NO + M >>> NO2 + M	1.13D-13	8.39D-48
13	O + NO2 >>> NO + O2	5.12D-12	6.27D-53
14	O + NO2 + M >>> NO3 + M	7.07D-14	5.66D-24
15	HO + HO >>> H2O + O	1.09D-12	9.77D-27
16	O2 + 2*NO >>> 2*NO2	2.75D-38	3.88D-35

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	6.500D 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	1.410D 17	3.000D 09	1.000D 06	1.000D 11
0.50	6.500D 08	6.395D 09	1.961D 06	6.905D 09	4.300D 12	1.410D 17	3.000D 09	9.923D 05	1.000D 11
1.00	6.500D 08	6.489D 09	1.928D 06	6.811D 09	4.300D 12	1.410D 17	3.000D 09	9.845D 05	1.000D 11
1.50	6.500D 08	6.582D 09	1.899D 06	6.718D 09	4.300D 12	1.410D 17	3.000D 09	9.766D 05	1.000D 11
2.00	6.500D 08	6.673D 09	1.875D 06	6.627D 09	4.300D 12	1.410D 17	3.000D 09	9.687D 05	1.000D 11
2.50	6.500D 08	6.763D 09	1.856D 06	6.537D 09	4.300D 12	1.410D 17	3.000D 09	9.608D 05	1.000D 11
3.00	6.500D 08	6.852D 09	1.840D 06	6.448D 09	4.299D 12	1.410D 17	3.000D 09	9.528D 05	1.000D 11
3.50	6.500D 08	6.940D 09	1.828D 06	6.360D 09	4.299D 12	1.410D 17	3.000D 09	9.448D 05	1.000D 11
4.00	6.500D 08	7.026D 09	1.820D 06	6.274D 09	4.299D 12	1.410D 17	3.000D 09	9.368D 05	1.000D 11
4.50	6.500D 08	7.111D 09	1.814D 06	6.189D 09	4.299D 12	1.410D 17	3.000D 09	9.287D 05	1.000D 11
5.00	6.500D 08	7.195D 09	1.812D 06	6.105D 09	4.299D 12	1.410D 17	3.000D 09	9.206D 05	1.000D 11
5.50	6.500D 08	7.278D 09	1.812D 06	6.022D 09	4.299D 12	1.410D 17	3.000D 09	9.125D 05	1.000D 11
6.00	6.500D 08	7.360D 09	1.814D 06	5.940D 09	4.299D 12	1.410D 17	3.000D 09	9.043D 05	1.000D 11
6.50	6.500D 08	7.441D 09	1.819D 06	5.859D 09	4.299D 12	1.410D 17	3.000D 09	8.962D 05	1.000D 11
7.00	6.500D 08	7.521D 09	1.826D 06	5.780D 09	4.299D 12	1.410D 17	3.000D 09	8.880D 05	1.000D 11
7.50	6.500D 08	7.599D 09	1.836D 06	5.701D 09	4.299D 12	1.410D 17	3.000D 09	8.798D 05	1.000D 11
8.00	6.500D 03	7.677D 09	1.847D 06	5.623D 09	4.299D 12	1.410D 17	3.000D 09	8.717D 05	1.000D 11
8.50	6.500D 08	7.753D 09	1.859D 06	5.547D 09	4.299D 12	1.410D 17	3.000D 09	8.635D 05	1.000D 11
9.00	6.500D 08	7.828D 09	1.874D 06	5.472D 09	4.298D 12	1.410D 17	3.000D 09	8.553D 05	1.000D 11
9.50	6.500D 08	7.903D 09	1.890D 06	5.397D 09	4.298D 12	1.410D 17	3.000D 09	8.471D 05	1.000D 11
10.00	6.500D 08	7.976D 09	1.908D 06	5.324D 09	4.298D 12	1.410D 17	3.000D 09	8.389D 05	1.000D 11

25 km HNO_3, N_2O_5, O, 300°K

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	3.27D-03	5.94D-14
2	2*NO3 >>> 2*NO2 + O2	2.41D-16	1.75D-58
3	NO2 + NO3 >>> NO2 + NO + O2	8.21D-15	4.92D-35
4	NO3 + NO >>> 2*NO2	1.90D-11	6.98D-29
5	NO + O3 >>> NO2 + O2	1.67D-14	2.85D-49
6	NO2 + O3 >>> NO3 + O2	3.41D-17	2.00D-34
7	HNO3 + M >>> HO + NO2 + M	4.01D-21	1.30D-12
8	HNO3 + HO >>> H2O + NO3	8.00D-14	1.69D-27
9	O + O + M >>> O2 + M	1.23D-15	5.48D-58
10	O + O2 + M >>> O3 + M	3.42D-16	2.74D-09
11	O + O3 >>> 2*O2	8.90D-15	0.0
12	O + NO + M >>> NO2 + M	6.40D-14	2.51D-38
13	O + NO2 >>> NO + O2	6.25D-12	3.73D-46
14	O + NO2 + M >>> NO3 + M	5.89D-14	4.71D-24
15	HO + HO >>> H2O + O	1.57D-12	4.63D-24
16	O2 + 2*NO >>> 2*NO2	1.93D-38	2.26D-31

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	6.500D 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	1.180D 17	3.000D 09	1.000D 06	1.000D 11
0.50	6.489D 08	6.548D 09	3.358D 06	6.753D 09	4.300D 12	1.180D 17	3.000D 09	9.959D 05	1.000D 11
1.00	6.479D 08	6.787D 09	4.655D 06	6.514D 09	4.300D 12	1.180D 17	3.000D 09	9.916D 05	1.000D 11
1.50	6.468D 08	7.019D 09	5.898D 06	6.284D 09	4.299D 12	1.180D 17	3.000D 09	9.872D 05	1.000D 11
2.00	6.458D 08	7.242D 09	7.096D 06	6.062D 09	4.299D 12	1.180D 17	3.000D 09	9.827D 05	1.000D 11
2.50	6.447D 08	7.457D 09	8.255D 06	5.847D 09	4.299D 12	1.180D 17	3.000D 09	9.780D 05	1.000D 11
3.00	6.437D 08	7.665D 09	9.380D 06	5.641D 09	4.299D 12	1.180D 17	3.000D 09	9.732D 05	1.000D 11
3.50	6.426D 08	7.865D 09	1.048D 07	5.441D 09	4.298D 12	1.180D 17	3.000D 09	9.684D 05	1.000D 11
4.00	6.416D 08	8.059D 09	1.155D 07	5.248D 09	4.298D 12	1.180D 17	3.000D 09	9.634D 05	1.000D 11
4.50	6.405D 08	8.246D 09	1.260D 07	5.063D 09	4.298D 12	1.180D 17	3.000D 09	9.584D 05	1.000D 11
5.00	6.395D 08	8.426D 09	1.364D 07	4.883D 09	4.298D 12	1.180D 17	3.000D 09	9.532D 05	1.000D 11
5.50	6.384D 08	8.600D 09	1.466D 07	4.710D 09	4.298D 12	1.180D 17	3.000D 09	9.480D 05	1.000D 11
6.00	6.374D 08	8.768D 09	1.567D 07	4.544D 09	4.298D 12	1.180D 17	3.000D 09	9.427D 05	1.000D 11
6.50	6.363D 08	8.930D 09	1.667D 07	4.383D 09	4.297D 12	1.180D 17	3.000D 09	9.373D 05	1.000D 11
7.00	6.353D 08	9.086D 09	1.766D 07	4.227D 09	4.297D 12	1.180D 17	3.000D 09	9.319D 05	1.000D 11
7.50	6.343D 08	9.237D 09	1.865D 07	4.078D 09	4.297D 12	1.180D 17	3.000D 09	9.264D 05	1.000D 11
8.00	6.332D 08	9.383D 09	1.963D 07	3.933D 09	4.297D 12	1.180D 17	3.000D 09	9.209D 05	1.000D 11
8.50	6.322D 08	9.523D 09	2.062D 07	3.793D 09	4.297D 12	1.180D 17	3.000D 09	9.153D 05	1.000D 11
9.00	6.312D 08	9.659D 09	2.160D 07	3.659D 09	4.297D 12	1.180D 17	3.000D 09	9.096D 05	1.000D 11
9.50	6.302D 08	9.790D 09	2.258D 07	3.529D 09	4.297D 12	1.180D 17	3.000D 09	9.039D 05	1.000D 11
10.00	6.291D 08	9.916D 09	2.357D 07	3.404D 09	4.296D 12	1.180D 17	3.000D 09	8.982D 05	1.000D 11

25 km HNO_3, N_2O_5, O, 400°K

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N205 + M >>> NO2 +NO3 + M	1.33D 01	2.17D-14
2	2*NO3 >>> 2*NO2 + O2	1.86D-15	2.85D-54
3	NO2 + NO3 >>> NO2 + NO + O2	1.89D-14	1.63D-35
4	NO3 + NO >>> 2*NO2	1.90D-11	1.00D-24
5	NO + O3 >>> NO2 + O2	5.60D-14	5.39D-40
6	NO2 + O3 >>> NO3 + O2	2.62D-16	5.96D-29
7	HNO3 + M >>> HO + NO2 + M	1.20D-12	4.75D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	3.49D-24
9	O + O + M >>> O2 + M	4.36D-16	5.06D-48
10	O + O2 + M >>> O3 + M	1.68D-16	2.82D-05
11	O + O3 >>> 2*O2	6.05D-14	6.81D-66
12	O + NO + M >>> NO2 + [illegible]	2.95D-14	1.65D-26
13	O + NO2 >>> [illegible]	8.03D-12	1.10D-37
14	[illegible]	4.42D-14	3.54D-24
	[illegible]	2.50D-12	1.02D-20
	[illegible] NO >>> 2*NO2	1.24D-38	1.09D-26

HAPP RESIDENCE TIME STUDY

TIME(S)	N205	N02	N03	NO	O3	O2	HNO3	HO	H2O
0.0	6.500D 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	8.840D 16	3.000D 09	1.000D 06	1.000D 11
0.50	8.480D 05	7.804D 09	6.216D 08	6.175D 09	4.299D 12	8.840D 16	3.000D 09	9.983D 05	1.000D 11
1.00	9.341D 03	8.565D 09	5.936D 08	5.444D 09	4.298D 12	8.840D 16	3.000D 09	9.964D 05	1.000D 11
1.50	8.561D 03	9.231D 09	5.703D 08	4.801D 09	4.298D 12	8.840D 16	3.000D 09	9.943D 05	1.000D 11
2.00	8.811D 03	9.816D 09	5.516D 08	4.234D 09	4.297D 12	8.840D 16	3.000D 09	9.921D 05	1.000D 11
2.50	9.026D 03	1.033D 10	5.366D 08	3.736D 09	4.297D 12	8.840D 16	3.000D 09	9.898D 05	1.000D 11
3.00	9.217D 03	1.078D 10	5.248D 08	3.296D 09	4.296D 12	8.840D 16	3.000D 09	9.873D 05	1.000D 11
3.50	9.391D 03	1.118D 10	5.157D 08	2.909D 09	4.296D 12	8.840D 16	3.000D 09	9.848D 05	1.000D 11
4.00	9.555D 03	1.153D 10	5.087D 08	2.567D 09	4.296D 12	8.840D 16	3.000D 09	9.822D 05	1.000D 11
4.50	9.713D 03	1.183D 10	5.036D 08	2.266D 09	4.295D 12	8.840D 16	3.000D 09	9.795D 05	1.000D 11
5.00	9.866D 03	1.210D 10	5.002D 08	2.000D 09	4.295D 12	8.840D 16	3.000D 09	9.767D 05	1.000D 11
5.50	1.002D 04	1.234D 10	4.981D 08	1.766D 09	4.295D 12	8.840D 16	3.000D 09	9.739D 05	1.000D 11
6.00	1.017D 04	1.255D 10	4.972D 08	1.559D 09	4.295D 12	8.840D 16	3.000D 09	9.711D 05	1.000D 11
6.50	1.032D 04	1.273D 10	4.973D 08	1.376D 09	4.294D 12	8.840D 16	3.000D 09	9.682D 05	1.000D 11
7.00	1.047D 04	1.289D 10	4.984D 08	1.215D 09	4.294D 12	8.840D 16	3.000D 09	9.653D 05	1.000D 11
7.50	1.062D 04	1.303D 10	5.002D 08	1.073D 09	4.294D 12	8.840D 16	3.000D 09	9.624D 05	1.000D 11
8.00	1.078D 04	1.315D 10	5.027D 08	9.474D 08	4.294D 12	8.840D 16	3.000D 09	9.594D 05	1.000D 11
8.50	1.093D 04	1.326D 10	5.058D 08	8.366D 08	4.294D 12	8.840D 16	3.000D 09	9.564D 05	1.000D 11
9.00	1.109D 04	1.335D 10	5.095D 08	7.388D 08	4.294D 12	8.840D 16	3.000D 09	9.535D 05	1.000D 11
9.50	1.125D 04	1.344D 10	5.136D 08	6.524D 08	4.294D 12	8.840D 16	3.000D 09	9.505D 05	1.000D 11
10.00	1.141D 04	1.351D 10	5.181D 08	5.762D 08	4.294D 12	8.840D 16	3.000D 09	9.475D 05	1.000D 11

25 km HNO_3, N_2O_5, O, 550°K

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N205 + M >>> NO2 +NO3 + M	1.10D 04	8.79D-15
2	2*NO3 >>> 2*NO2 + O2	9.88D-15	7.98D-51
3	NO2 + NO3 >>> NO2 + NO + O2	3.73D-14	6.64D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.54D-21
5	NO + O3 >>> NO2 + O2	1.50D-13	2.09D-32
6	NO2 + O3 >>> NO3 + O2	1.40D-15	1.81D-24
7	HNO3 + M >>> HO + NO2 + M	7.06D-06	1.56D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	1.80D-21
9	O + O + M >>> O2 + M	1.72D-16	9.45D-31
10	O + O2 + M >>> O3 + M	8.61D-17	4.97D-02
11	O + O3 >>> 2*O2	2.90D-13	3.43D-51
12	O + NO + M >>> NO2 + M	1.44D-14	7.09D-17
13	O + NO2 >>> NO + O2	9.85D-12	9.33D-31
14	O + NO2 + M >>> NO3 + M	3.21D-14	2.57D-24
15	HO + HO >>> H2O + O	3.65D-12	5.56D-18
16	O2 + 2*NO >>> 2*NO2	8.65D-39	6.75D-23

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	6.500D 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	6.430D 16	3.000D 09	1.000D 06	1.000D 11
0.50	4.175D 00	8.163D 09	6.391D 08	5.800D 09	4.240D 12	6.430D 16	3.000D 09	1.010D 06	1.000D 11
1.00	4.411D 00	8.685D 09	6.346D 08	5.282D 09	4.199D 12	6.430D 16	3.000D 09	1.020D 06	1.000D 11
1.50	4.564D 00	8.997D 09	6.338D 08	4.971D 09	4.159D 12	6.430D 16	3.000D 09	1.030D 06	1.000D 11
2.00	4.670D 00	9.187D 09	6.351D 08	4.780D 09	4.120D 12	6.430D 16	3.000D 09	1.040D 06	1.000D 11
2.50	4.746D 00	9.303D 09	6.374D 08	4.662D 09	4.082D 12	6.430D 16	3.000D 09	1.050D 06	1.000D 11
3.00	4.802D 00	9.373D 09	6.402D 08	4.589D 09	4.044D 12	6.430D 16	3.000D 09	1.059D 06	1.000D 11
3.50	4.846D 00	9.415D 09	6.431D 08	4.544D 09	4.007D 12	6.430D 16	3.000D 09	1.069D 06	1.000D 11
4.00	4.880D 00	9.440D 09	6.459D 08	4.517D 09	3.971D 12	6.430D 16	3.000D 09	1.079D 06	1.000D 11
4.50	4.907D 00	9.453D 09	6.485D 08	4.501D 09	3.935D 12	6.430D 16	3.000D 09	1.089D 06	1.000D 11
5.00	4.928D 00	9.460D 09	6.509D 08	4.491D 09	3.900D 12	6.430D 16	3.000D 09	1.099D 06	1.000D 11
5.50	4.945D 00	9.463D 09	6.529D 08	4.486D 09	3.865D 12	6.430D 16	3.000D 09	1.109D 06	1.000D 11
6.00	4.958D 00	9.463D 09	6.547D 08	4.484D 09	3.831D 12	6.430D 16	3.000D 09	1.118D 06	1.000D 11
6.50	4.968D 00	9.462D 09	6.561D 08	4.484D 09	3.797D 12	6.430D 16	3.000D 09	1.128D 06	1.000D 11
7.00	4.976D 00	9.460D 09	6.572D 08	4.485D 09	3.764D 12	6.430D 16	3.000D 09	1.138D 06	1.000D 11
7.50	4.980D 00	9.457D 09	6.580D 08	4.487D 09	3.731D 12	6.430D 16	3.000D 09	1.148D 06	1.000D 11
8.00	4.983D 00	9.454D 09	6.585D 08	4.490D 09	3.699D 12	6.430D 16	3.000D 09	1.157D 06	1.000D 11
8.50	4.983D 00	9.451D 09	6.587D 08	4.492D 09	3.668D 12	6.430D 16	3.000D 09	1.167D 06	1.000D 11
9.00	4.981D 00	9.448D 09	6.587D 08	4.495D 09	3.637D 12	6.430D 16	3.000D 09	1.177D 06	1.000D 11
9.50	4.977D 00	9.445D 09	6.584D 08	4.498D 09	3.606D 12	6.430D 16	3.000D 09	1.187D 06	1.000D 11
10.00	4.972D 00	9.443D 09	6.579D 08	4.502D 09	3.576D 12	6.430D 16	3.000D 09	1.196D 06	1.000D 11

25 km HNO_3, N_2O_5, O, 600°K

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	4.80D 04	7.07D-15
2	2*NO3 >>> 2*NO2 + O2	1.43D-14	4.66D-50
3	NO2 + NO3 >>> NO2 + NO + O2	4.34D-14	5.43D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.45D-20
5	NO + O3 >>> NO2 + O2	1.87D-13	1.02D-30
6	NO2 + O3 >>> NO3 + O2	2.02D-15	1.79D-23
7	HNO3 + M >>> HO + NO2 + M	2.10D-04	1.15D-13
8	HNO3 + HO >>> H2O + NO3	8.00D-14	7.21D-21
9	O + O + M >>> O2 + M	1.37D-16	6.30D-27
10	O + O2 + M >>> O3 + M	7.31D-17	2.58D-01
11	O + O3 >>> 2*O2	4.11D-13	6.34D-48
12	O + NO + M >>> NO2 + M	1.21D-14	9.65D-15
13	O + NO2 >>> NO + O2	1.03D-11	3.23D-29
14	O + NO2 + M >>> NO3 + M	2.95D-14	2.36D-24
15	HO + HO >>> H2O + O	3.97D-12	2.26D-17
16	O2 + 2*NO >>> 2*NO2	7.98D-39	4.63D-22

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	6.500D 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	5.890D 16	3.000D 09	1.000D 06	1.000D 11
0.50	5.473D-01	5.758D 09	6.460D 08	8.199D 09	3.929D 12	5.890D 16	3.000D 09	1.314D 06	1.000D 11
1.00	4.266D-01	4.643D 09	6.243D 08	9.335D 09	3.664D 12	5.890D 16	2.999D 09	1.629D 06	1.000D 11
1.50	3.740D-01	4.270D 09	5.951D 08	9.737D 09	3.431D 12	5.890D 16	2.999D 09	1.943D 06	1.000D 11
2.00	3.433D-01	4.134D 09	5.644D 08	9.905D 09	3.224D 12	5.890D 16	2.999D 09	2.257D 06	1.000D 11
2.50	3.199D-01	4.070D 09	5.342D 08	9.999D 09	3.037D 12	5.890D 16	2.998D 09	2.571D 06	1.000D 11
3.00	2.995D-01	4.031D 09	5.050D 08	1.007D 10	2.869D 12	5.890D 16	2.998D 09	2.885D 06	1.000D 11
3.50	2.809D-01	4.002D 09	4.771D 08	1.013D 10	2.717D 12	5.890D 16	2.998D 09	3.199D 06	1.000D 11
4.00	2.636D-01	3.978D 09	4.505D 08	1.018D 10	2.578D 12	5.890D 16	2.997D 09	3.512D 06	1.000D 11
4.50	2.475D-01	3.956D 09	4.252D 08	1.022D 10	2.452D 12	5.890D 16	2.997D 09	3.826D 06	1.000D 11
5.00	2.325D-01	3.936D 09	4.014D 08	1.027D 10	2.337D 12	5.890D 16	2.997D 09	4.139D 06	1.000D 11
5.50	2.184D-01	3.918D 09	3.788D 08	1.031D 10	2.230D 12	5.890D 16	2.997D 09	4.452D 06	1.000D 11
6.00	2.053D-01	3.902D 09	3.575D 08	1.035D 10	2.133D 12	5.890D 16	2.996D 09	4.765D 06	1.000D 11
6.50	1.930D-01	3.886D 09	3.375D 08	1.038D 10	2.042D 12	5.890D 16	2.996D 09	5.078D 06	1.000D 11
7.00	1.815D-01	3.871D 09	3.167D 08	1.042D 10	1.959D 12	5.890D 16	2.996D 09	5.391D 06	1.000D 11
7.50	1.709D-01	3.858D 09	3.010D 08	1.045D 10	1.881D 12	5.890D 16	2.995D 09	5.703D 06	1.000D 11
8.00	1.609D-01	3.845D 09	2.845D 08	1.048D 10	1.809D 12	5.890D 16	2.995D 09	6.016D 06	1.000D 11
8.50	1.516D-01	3.832D 09	2.689D 08	1.051D 10	1.742D 12	5.890D 16	2.995D 09	6.328D 06	1.000D 11
9.00	1.430D-01	3.821D 09	2.544D 08	1.053D 10	1.679D 12	5.890D 16	2.994D 09	6.640D 06	1.000D 11
9.50	1.349D-01	3.810D 09	2.407D 08	1.056D 10	1.621D 12	5.890D 16	2.994D 09	6.952D 06	1.000D 11
10.00	1.274D-01	3.799D 09	2.280D 08	1.058D 10	1.565D 12	5.890D 16	[illegible]994D 09	7.264D 06	1.000D 11

25 km, HNO_3, N_2O_5, O, 700°K

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	4.80D 05	4.94D-15
2	2*NO3 >>> 2*NO2 + O2	2.57D-14	7.44D-49
3	NO2 + NO3 >>> NO2 + NO + O2	5.51D-14	3.97D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	2.23D-19
5	NO + O3 >>> NO2 + O2	2.65D-13	4.54D-28
6	NO2 + O3 >>> NO3 + O2	3.62D-15	6.56D-22
7	HNO3 + M >>> HO + NO2 + M	4.01D-02	6.70D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	6.38D-20
9	O + O + M >>> O2 + M	9.50D-17	6.21D-21
10	O + O2 + M >>> O3 + M	5.55D-17	3.36D 00
11	O + O3 >>> 2*O2	7.11D-13	8.63D-43
12	O + NO + M >>> NO2 + M	9.01D-15	2.14D-11
13	O + NO2 >>> NO + O2	1.11D-11	8.50D-27
14	O + NO2 + M >>> NO3 + M	2.53D-14	2.02D-24
15	HO + HO >>> H2O + O	4.53D-12	2.04D-16
16	O2 + 2*NO >>> 2*NO2	7.04D-39	9.37D-21

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	6.500D 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	5.000D 16	3.000D 09	1.000D 06	1.000D 11
0.50	2.432D-03	3.847D 08	6.152D 08	1.366D 10	1.266D 12	5.000D 16	2.940D 09	6.049D 07	9.999D 10
1.00	1.779D-03	3.178D 08	5.449D 08	1.386D 10	8.002D 11	5.000D 16	2.882D 09	1.188D 08	9.998D 10
1.50	1.602D-03	3.241D 08	4.810D 08	1.397D 10	6.071D 11	5.001D 16	2.825D 09	1.758D 08	9.997D 10
2.00	1.451D-03	3.330D 08	4.239D 08	1.408D 10	4.904D 11	5.001D 16	2.769D 09	2.316D 08	9.996D 10
2.50	1.306D-03	3.406D 08	3.731D 08	1.417D 10	4.112D 11	5.001D 16	2.714D 09	2.862D 08	9.996D 10
3.00	1.170D-03	3.469D 08	3.281D 08	1.427D 10	3.540D 11	5.001D 16	2.660D 09	3.396D 08	9.995D 10
3.50	1.043D-03	3.521D 08	2.883D 08	1.435D 10	3.106D 11	5.001D 16	2.607D 09	3.917D 08	9.995D 10
4.00	9.273D-04	3.564D 08	2.531D 08	1.444D 10	2.766D 11	5.001D 16	2.556D 09	4.425D 08	9.994D 10
4.50	8.221D-04	3.601D 08	2.221D 08	1.451D 10	2.493D 11	5.001D 16	2.505D 09	4.922D 08	9.994D 10
5.00	7.273D-04	3.631D 08	1.949D 08	1.459D 10	2.268D 11	5.001D 16	2.455D 09	5.406D 08	9.994D 10
5.50	6.424D-04	3.657D 08	1.709D 08	1.466D 10	2.080D 11	5.001D 16	2.406D 09	5.878D 08	9.994D 10
6.00	5.667D-04	3.679D 08	1.499D 08	1.473D 10	1.921D 11	5.001D 16	2.359D 09	6.338D 08	9.994D 10
6.50	4.994D-04	3.698D 08	1.314D 08	1.479D 10	1.784D 11	5.001D 16	2.312D 09	6.785D 08	9.993D 10
7.00	4.399D-04	3.714D 08	1.152D 08	1.485D 10	1.665D 11	5.001D 16	2.266D 09	7.221D 08	9.993D 10
7.50	3.873D-04	3.729D 08	1.011D 08	1.491D 10	1.560D 11	5.001D 16	2.221D 09	7.645D 08	9.993D 10
8.00	3.409D-04	3.741D 08	8.866D 07	1.496D 10	1.468D 11	5.001D 16	2.177D 09	8.056D 08	9.993D 10
8.50	3.001D-04	3.753D 08	7.781D 07	1.502D 10	1.386D 11	5.001D 16	2.134D 09	8.456D 08	9.993D 10
9.00	2.643D-04	3.764D 08	6.832D 07	1.507D 10	1.312D 11	5.001D 16	2.091D 09	8.845D 08	9.993D 10
9.50	2.329D-04	3.774D 08	6.003D 07	1.511D 10	1.246D 11	5.001D 16	2.050D 09	9.222D 08	9.993D 10
10.00	2.053D-04	3.784D 08	5.279D 07	1.516D 10	1.186D 11	5.001D 16	2.009D 09	9.587D 08	9.993D 10

25 km, HNO_3, N_2O_5, O, $800^{o}K$

R-NUM	REACTION	FORWARD RATE	BACKWARD RATE
1	N2O5 + M >>> NO2 +NO3 + M	2.65D 06	3.70D-15
2	2*NO3 >>> 2*NO2 + O2	3.98D-14	5.95D-48
3	NO2 + NO3 >>> NO2 + NO + O2	6.59D-14	3.13D-36
4	NO3 + NO >>> 2*NO2	1.90D-11	1.74D-18
5	NO + O3 >>> NO2 + O2	3.43D-13	4.42D-26
6	NO2 + O3 >>> NO3 + O2	5.61D-15	9.78D-21
7	HNO3 + M >>> HO + NO2 + M	1.90D 00	4.20D-14
8	HNO3 + HO >>> H2O + NO3	8.00D-14	3.28D-19
9	O + O + M >>> O2 + M	7.08D-17	1.87D-16
10	O + O2 + M >>> O3 + M	4.43D-17	2.26D 01
11	O + O3 >>> 2*O2	1.07D-12	6.11D-39
12	O + NO + M >>> NO2 + M	7.[illegible]D-15	6.78D-09
13	O + NO2 >>> NO + O2	1.17D-11	5.55D-25
14	O + NO2 + M >>> NO3 + M	2.21D-14	1.77D-24
15	HO + HO >>> H2O + O	5.00D-12	1.06D-15
16	O2 + 2*NO >>> 2*NO2	6.40D-39	8.78D-20

HAPP RESIDENCE TIME STUDY

TIME(S)	N2O5	NO2	NO3	NO	O3	O2	HNO3	HO	H2O
0.0	6.5000 08	6.300D 09	2.000D 06	7.000D 09	4.300D 12	4.400D 16	3.000D 09	1.000D 06	1.000D 11
0.50	1.048D-04	1.270D 08	5.909D 08	1.572D 10	2.141D 11	4.400D 16	1.161D 09	1.833D 09	9.985D 10
1.00	6.697D-05	9.414D 07	5.094D 08	1.655D 10	1.792D 11	4.401D 16	4.495D 08	2.519D 09	9.973D 10
1.50	4.751D-05	7.798D 07	4.362D 08	1.691D 10	1.537D 11	4.401D 16	1.740D 08	2.759D 09	9.964D 10
2.00	3.657D-05	7.031D 07	3.724D 08	1.709D 10	1.344D 11	4.401D 16	6.736D 07	2.827D 09	9.957D 10
2.50	2.956D-05	6.668D 07	3.175D 08	1.719D 10	1.193D 11	4.401D 16	2.608D 07	2.828D 09	9.950D 10
3.00	2.450D-05	6.486D 07	2.704D 08	1.726D 10	1.072D 11	4.401D 16	1.010D 07	2.804D 09	9.945D 10
3.50	2.052D-05	6.382D 07	2.303D 08	1.730D 10	9.728D 10	4.401D 16	3.910D 06	2.771D 09	9.940D 10
4.00	1.727D-05	6.308D 07	1.960D 08	1.734D 10	8.899D 10	4.401D 16	1.516D 06	2.736D 09	9.936D 10
4.50	1.455D-05	6.246D 07	1.669D 08	1.737D 10	8.198D 10	4.401D 16	5.891D 05	2.700D 09	9.933D 10
5.00	1.227D-05	6.186D 07	1.420D 08	1.740D 10	7.598D 10	4.401D 16	2.303D 05	2.664D 09	9.930D 10
5.50	1.035D-05	6.131D 07	1.209D 08	1.742D 10	7.078D 10	4.401D 16	9.135D 04	2.630D 09	9.927D 10
6.00	8.736D-06	6.075D 07	1.030D 08	1.744D 10	6.623D 10	4.401D 16	3.752D 04	2.595D 09	9.924D 10
6.50	7.375D-06	6.021D 07	8.771D 07	1.745D 10	6.223D 10	4.401D 16	1.663D 04	2.562D 09	9.922D 10
7.00	6.230D-06	5.970D 07	7.473D 07	1.747D 10	5.867D 10	4.401D 16	8.504D 03	2.530D 09	9.919D 10
7.50	5.268D-06	5.921D 07	6.371D 07	1.748D 10	5.549D 10	4.401D 16	5.314D 03	2.498D 09	9.917D 10
8.00	4.459D-06	5.876D 07	5.434D 07	1.749D 10	5.264D 10	4.401D 16	4.039D 03	2.467D 09	9.916D 10
8.50	3.778D-06	5.833D 07	4.638D 07	1.750D 10	5.006D 10	4.401D 16	3.506D 03	2.437D 09	9.914D 10
9.00	3.206D-06	5.795D 07	3.962D 07	1.750D 10	4.771D 10	4.401D 16	3.263D 03	2.408D 09	9.912D 10
9.50	2.724D-06	5.759D 07	3.387D 07	1.751D 10	4.558D 10	4.401D 16	3.134D 03	2.379D 09	9.911D 10
10.00	2.318D-06	5.727D 07	2.899D 07	1.752D 10	4.362D 10	4.401D 16	3.052D 03	2.352D 09	9.910D 10

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